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INFLUENCE OF GRÜNWALD-LETNIKOV TIME AND SPACE TEMPERATURE DERIVATIVE ON HEAT DISTRIBUTION

Summary

In this paper the new thermal model called Dual-Phase-Lag model has been investigated. This method is reasonable for nanometric structures which are more and more popular nowadays. However, during its numerical implementation, some problems can occur. Moreover, the simulation process can take a long period of time. Thus, it is needed to find some approximation scheme of the Dual-Phase-Lag model, which provides highly accurate results and simultaneously reduces time of simulation. Due to these reasons, investigation presented in this paper focuses on the determination of the approximation of the Dual-Phase-Lag model based on the Grünwald-Letnikov derivative definition. Moreover, this approximation takes into consideration the time and space derivative at the same time.

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

1. Introduction

The continuous development of the technology and growth of customers demands and needs led to production totally new and modern electronic appliances. Moreover, new type of technical areas such as artificial intelligence, machine learning, deep learning or imagine recognition require more computational power and more efficient electronic structures. Many modern appliances offer different functions in one equipment. Simultaneously, the size of created devices is getting smaller and smaller. These reasons and requirements cause meaningful growth of devices' operation frequencies. It causes significant heat density generation inside the electronic structures what can lead to occurrence of thermal problems. The problems related to proper operation of the device can appear and, consequently, damages or malfunctions may take a place. Moreover, new designs of integrated circuit is needed and currently significantly bigger number of transistors is implemented inside these structures than in the past. Taking into account the small size, the big number of electronic component near each other, higher generation of the heat and increase of operation frequencies, it can occur that new phenomena can be observed. Thus, it is crucial to proper plan of modern electronic devices. One of the very important aspect during the designing and arrangement of electronic component processes is determination of the expected temperature distribution. It will allow avoiding the thermal malfunctions and increase the efficiency of devices operation. Due to these facts, new thermal solutions are needed.

The thermal methodology considered in this paper is called Dual-Phase-Lag (DPL). This thermal model was described and postulated by Tzou in 1995 [1]. The model contains two parameters related to the time lags, the heat flux and the temperature time lags. As it was described in [2], this approach is relevant for nanometric structures. Its mathematical form can be expressed by the following equation:

$$\begin{cases} c_v \frac{\partial T(x,y,t)}{\partial t} = -q\left(x,y,t\right) \\ q\left(x,y,t\right) + \tau_q \frac{\partial q(x,y,t)}{\partial t} = -k\nabla T\left(x,y,t\right) - k\tau_T \frac{\partial \nabla T(x,y,t)}{\partial t} \end{cases} \tag{1}$$

Moreover, as it was described in [3], the DPL model is a modification of the classical Fourier-Kirchhoff (FK) approach. Furthermore, the application of DPL model is relevant in the case of hyperbolic as well as parabolic cases. It causes that DPL model can have wide range of application. However, the form of DPL heat model is complex than the FK one, thus during its numerical application some difficulties can occur. First of all, the direct numerical implementation of DPL model produces huge computational complexity. Secondly, when the analyzed structure is characterized by a big number of different components, the bigger number of discretization nodes in simulation process is needed. It causes the increase of simulation time and demands more computational power. Taking into account these disadvantages, some approximation of the full DPL model, which will produce very accurate results and simultaneously the time of computation will be acceptable, is required. Thus, in this paper the determination of the approximation of DPL model is considered. This approximation is based on the definition of the Grünwald-Letnikov derivative. Moreover, the Grünwald-Letnikov definition has been applied to the time and space derivative of the temperature at the same time.

2. Grünwald-Letnikov Implementation

The form of the Grünwald-Letnikov fractional derivative can be described by the following formula [4]:

$$D^{\alpha}_{0,v}u(v) = \sum_{k=0}^{m-1} \frac{u^{(k)}(0)v^{-\alpha+k}}{\Gamma(-\alpha+k+1)} + \frac{1}{m-\alpha}\int_0^v (v-\tau)^{m-\alpha-1}u^{(m)}(\tau)d\tau \tag{2}$$

However, in order to use the Finite Difference Method to obtain the numerical solution of the temperature distribution in modern electronic structures, the following form of Grünwald-Letnikov derivatives for time and space order derivative have been delivered. Their mathematical forms present as follows:

$$D^{\alpha_t}_{0,t}u(t)_{GL} = \lim_{\Delta t\to 0}\frac{1}{\Delta t^{\alpha_t}}\sum_{k=0}^{N}(-1)^k\binom{\alpha_t}{k}u(t-k\Delta t) \tag{3}$$

$$D^{\alpha_x}_{0,x}u(x)_{GL} = \lim_{\Delta x\to 0}\frac{1}{\Delta x^{\alpha_x}}\sum_{k=0}^{N}(-1)^k\binom{\alpha_x}{k}u(x-k\Delta t+\frac{\alpha_x\Delta x}{2}) \tag{4}$$

Moreover, other simplicity has been applied. The binomial coefficient visible in equations above, has been replaced by its generalized form prepared for non-integer aguments using the special Γ function. The definition of the Grünwald-Letnikov derivatives has been applied to the following form of the FK equation:

$$c_v\frac{\partial T(\mathbf{x},t)}{\partial t} = k\Delta T(\mathbf{x},t) \tag{5}$$

using the following discrete forms to approximate the temperature time derivative and the Laplace operator of the temperature according to two below formulas, respectively:

$$\frac{\partial T(\mathbf{x},t)}{\partial t} = \frac{1}{\Delta t^{\alpha_t}}\sum_{k=0}^{round(\alpha_t,0)}(-1)^k\frac{\Gamma(\alpha_t+1)}{\Gamma(k+1)\Gamma(\alpha_t-k+1)}T(\mathbf{x},t-k\Delta t) \tag{6}$$

$$\Delta T(\mathbf{x},t) = \frac{1}{\Delta x^{\alpha_x}}\sum_{k=0}^{round(\alpha_x,0)}(-1)^k\frac{\Gamma(\alpha_x+1)}{\Gamma(k+1)\Gamma(\alpha_x-k+1)}T(\mathbf{x}-k\Delta x+\frac{\alpha_x\Delta x}{2},t) \tag{7}$$

Presented formulas have been employed to change the classical FK approach and to obtain the approximation scheme of the DPL model. Such modified FK model has been called by the Authors as space and time GL FK model.

All considerations presented in this paper has been tested using the two-dimensional square slab. Each dimension of this structure has 5 nm of length. Furthermore, the assumption that the heat flux was located in one of the corners of this slab has been made. Mentioned heat flux has been generated outside the structure. Moreover, on the edges neighbouring with the heated corner, the adiabatic boundary conditions have been imposed. On the other ones, the zero boundary conditions have been used. The investigated structure has been discretized in order to use the Finite Difference

Method to obtain the temperature distribution inside the the slab. The visualization of mentioned structure and the scheme of the structure nodes' numbering can be found in [5].

3. Simulations

The simulations focus on temperature distribution determination inside investigated nanosized electronic structure. The first analysis was related to the determination of proper values of the orders of derivatives for both the space and time variables. During the consideration, different values of the space as well as the time orders of derivatives have been tested using the space and time GL FK formula. Figures 1 - 3 present analyses related to the change of the value of the order of temperature time derivative and fixed value of the space one. In these figures, the order of the space temperature derivative was less than 2. Moreover, in all figures the FK results, marked by dark solid line, have been added to make the comparison and interpretation easier.

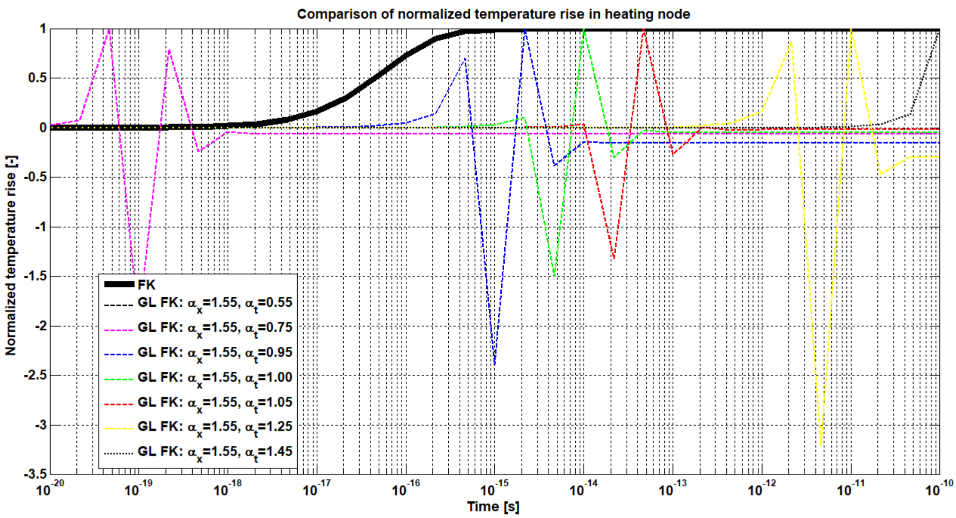

Fig. 1. Comparison of normalized temperature rises in heating node for temperature space derivative order equal to 1.55 and different orders of temperature time derivative

Figure 1 presents results obtained for space order α_x equal to 1.55 and the value of the time order derivative changes up to 1.45. As it is visible, obtained results strongly fluctuate. It can be suspected that considered cases are characterized by big numerical errors and do not provide proper results. Moreover negative values mean that the results are underestimated.

Figure 2 demonstrates the character of change of the temperature rises in the case when the space derivative order is equal to 1.75 and the order of the time derivative is changing similarly to the previous analyses. As it is shown, results seem to be more reliable than in the previous case. Two cases marked by pink and blue dashed lines are visible on the left side of the FK outputs. However, the character of obtained temperature rise in relation to analyzed parameter values is very similar.

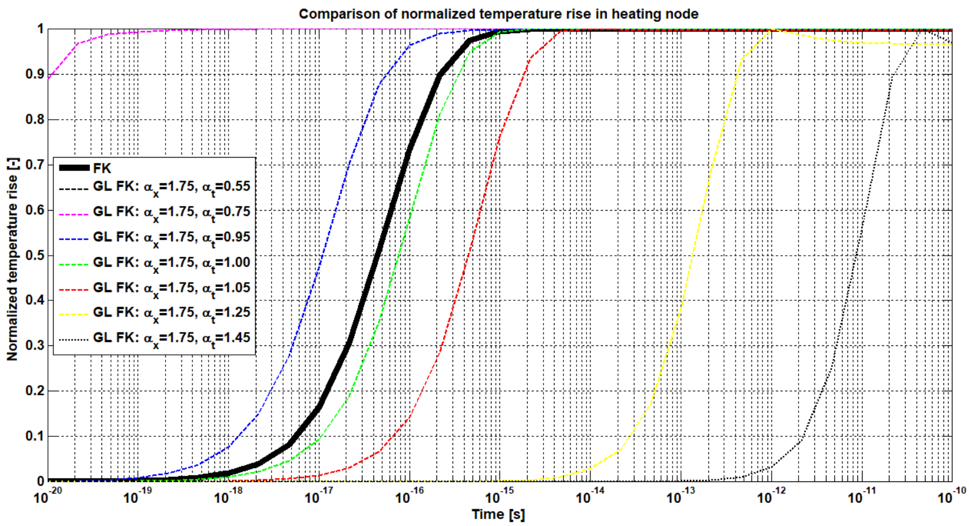

Fig. 2. Comparison of normalized temperature rises in heating node for temperature space derivative order equal to 1.75 and different orders of temperature time derivative

Figure 3 shows the dependence of the temperature rise in the case when space derivative order is equal to 1.95 and the time derivative order has the same values like in the previous cases. As it is observed, the character of change is also vary similar in all investigated cases. Two cases appear on the left side of the FK model while the remaining ones are visible on the right side. However, it can be observed that in the case of space derivative order closer to 2 the obtained results are located closer to the FK results. Thus, if the space derivative order value is closer to 2, the space and time GL FK model is less shifted in comparison to the original FK approach. Moreover, it occurred that for space derivative order approximately equal to 2 and for time derivative order equal to 1, the produced results are very similar to the FK model.

Next, analysis presented in Figure 4 focuses on the determination of the temperature rises for space and time GL FK model in the case when the space derivative order is equal to 2 and the time derivative order is changing. As it is demonstrated, for temperature time derivative smaller than 1 obtained results are placed on the left side of the FK model curve. Thus, they can be omitted in further analyses due to

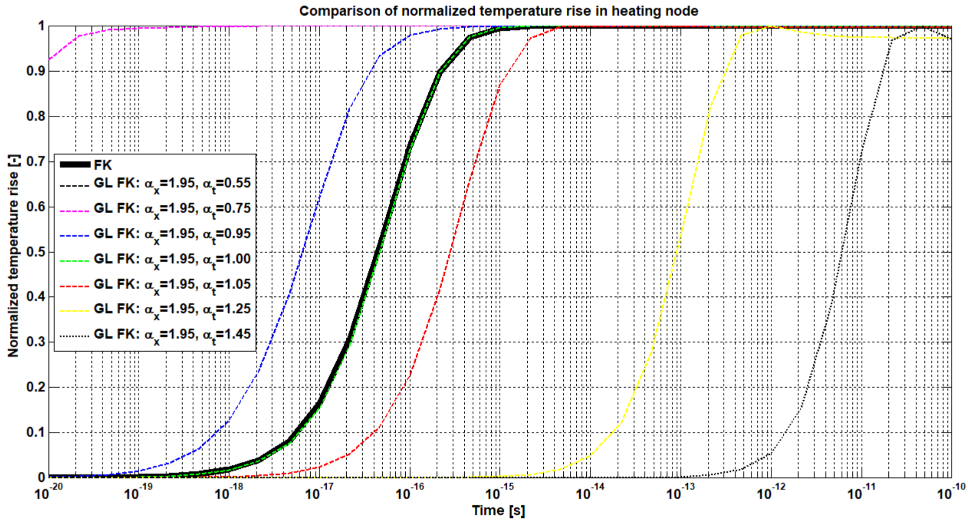

Fig. 3. Comparison of normalized temperature rises in heating node for temperature space derivative order equal to 1.95 and different orders of temperature time derivative

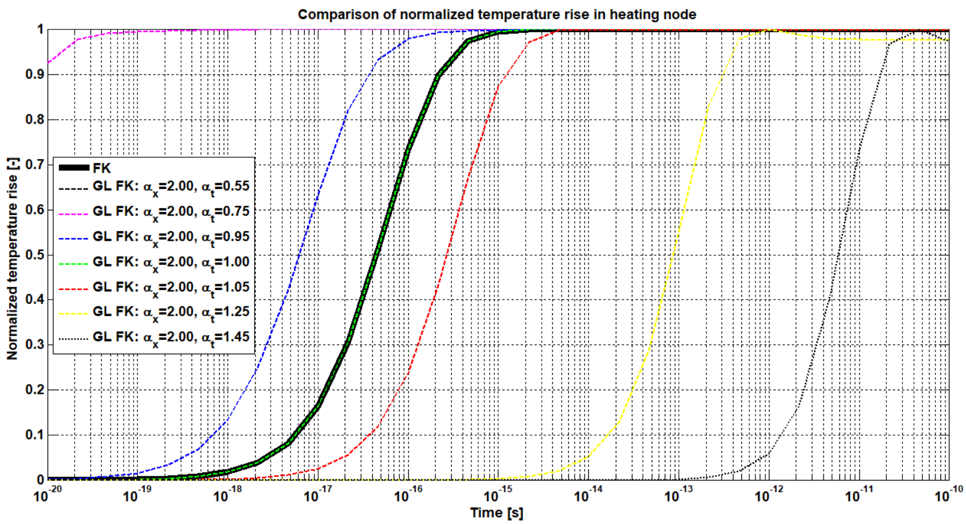

Fig. 4. Comparison of normalized temperature rises in heating node for temperature space derivative order equal to 2.00 and different orders of temperature time derivative

the fact that DPL model results are shifted to the right in relation to the FK one. As it can be observed, for the space derivative order equal to 2 and time derivative order equal to 1, the character of change of the temperature rises is exactly the same as in the case of the FK model. Furthermore, for higher value of the time derivative order, the bigger shift is observed.

On the other hand, results presented in Figures 5 - 7 have been obtained for the temperature space derivative order value higher than 2. As it is visible, in all demonstrated cases obtained results are characterized by significant errors. In Figure 5 the character of temperature rise change differs for different cases, while in Figure 6 and Figure 7 this dependence is not clearly visible and the steady state is characterized by the zero temperature rise, what, of course, is erroneous result. Thus, in further analyses, cases presented in Figures 5 - 7, i.e. values of the temperature space derivative order greater than 2, will not be investigated. Moreover, in order to obtain the DPL approximation using the space and time GL FK model, the cases of temperature time derivative order is smaller than 1, also will not be taken into consideration. Therefore, the investigations are based on results obtained for the space derivative order values from the interval $[1.56; 2.00]$ and for the time derivative order values belonging to the interval $[1.00; 1.49]$.

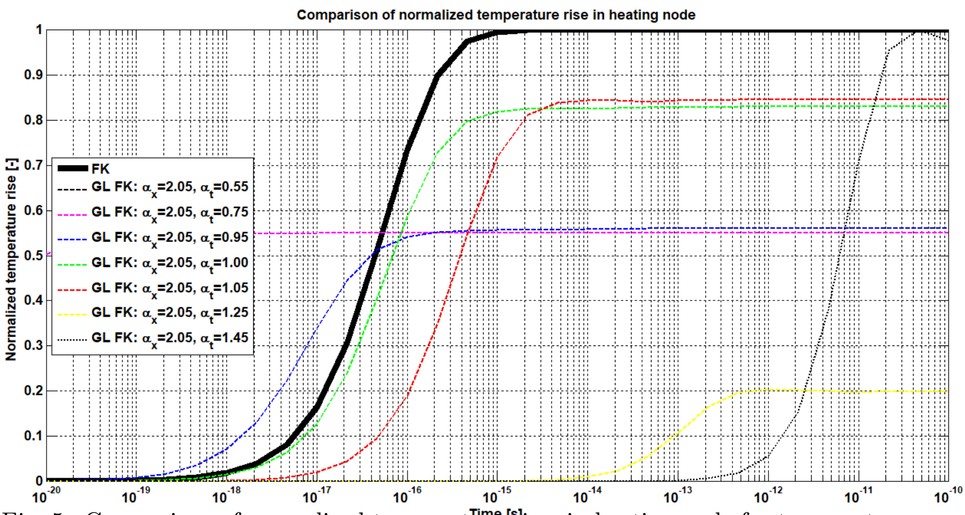

Fig. 5. Comparison of normalized temperature rises in heating node for temperature space derivative order equal to 2.05 and different orders of temperature time derivative

However, when the value of the temperature time derivative is greater than 1, the temperature rise has a specific character. Firstly, it behaves similarly to the classical temperature rise, however after reaching the maximal normalized temperature rise value, it decreases to the certain level. Moreover, this decrease is directly proportional to the increase of the value of order α_t. It means that the bigger value of α_t, the bigger decrease of the temperature rise after reaching the maximal point. Thus, the compensation of the temperature rise is needed. It has been carried out by replacing the decreased temperature rise values after reaching the maximal value by this maximum temperature rise value. After implementing the compensation procedure, the model has been called by the Authors as modified space and time GL FK model.

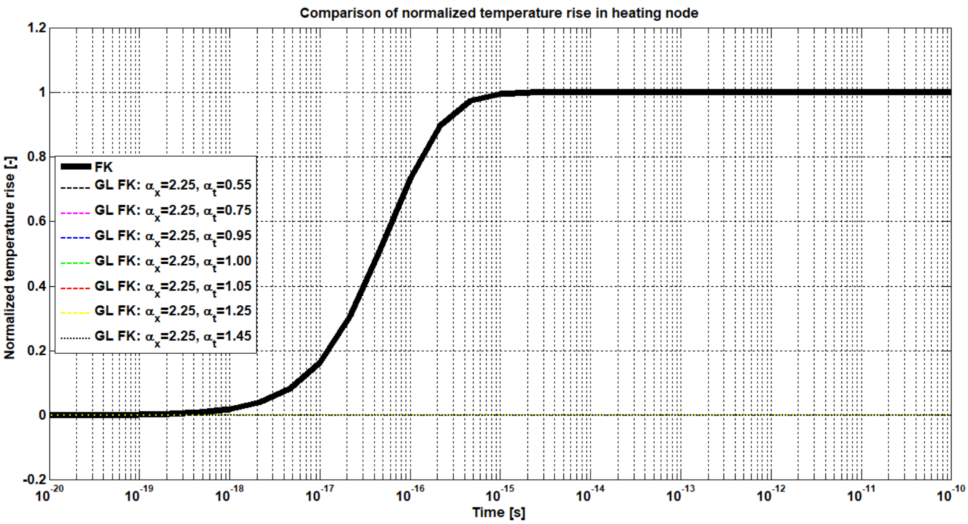

Fig. 6. Comparison of normalized temperature rises in heating node for temperature space derivative order equal to 2.25 and different orders of temperature time derivative

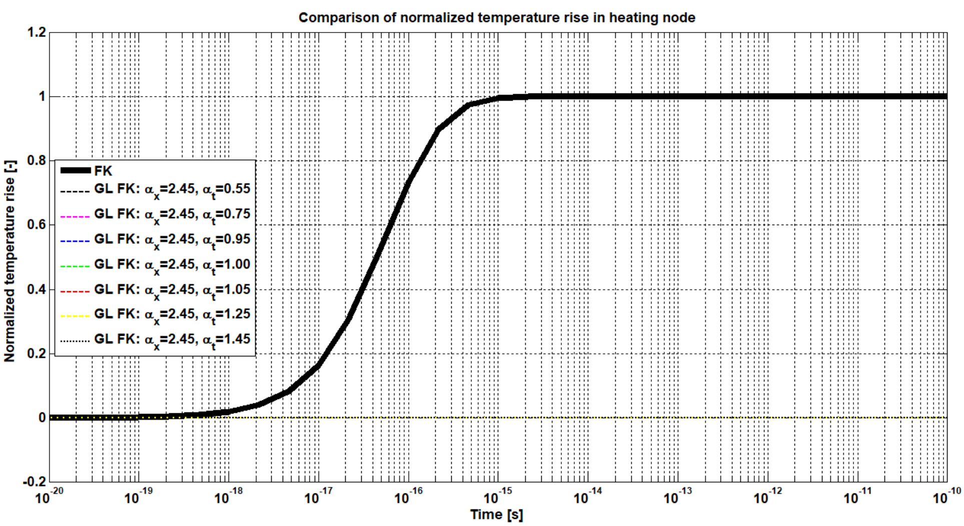

Fig. 7. Comparison of normalized temperature rises in heating node for temperature space derivative order equal to 2.45 and different orders of temperature time derivative

Figures 8 - 10 show the character of change of the temperature rise in the case when both space and time temperature derivative orders are from mentioned intervals. Figure 8 demonstrates temperature rises when the value of the space derivative order is constant, equal to 1.56, and value of the time derivative order is changing from 1.00 to 1.49.

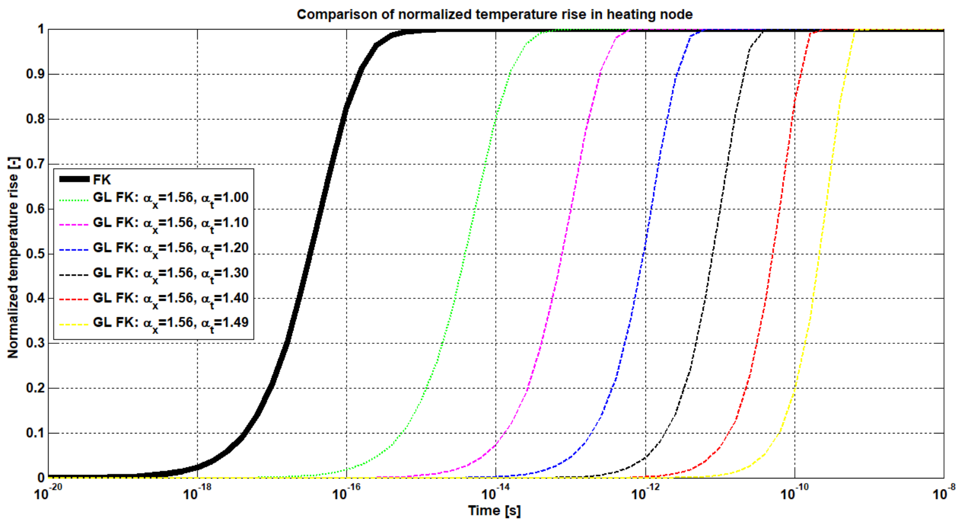

Fig. 8. Comparison of normalized temperature rises in heating node obtained using modified space and time GL FK models for temperature space derivative order equal to 1.56 and different orders of temperature time derivative

On the other hand, Figure 9 and Figure 10 present results obtained for different values of the time derivative order, while the value of the order of space derivative is equal to 1.75 and 2.00, respectively. As it is shown, all determined curves are observed on right side of the FK model. Moreover, character of these lines is very similar and visible shift is noticed. Furthermore, it can be concluded that for bigger value of the space derivative oder, the obtained results appear closer to the FK model output. On the contrary, for higher value of the time derivative order, the determined results are located further from the FK curve.

Based on the previous results, it is known that the behaviour of the temperature rises in heating nodes are similar for FK, DPL and modified space and time GL FK models. Thus, it is also worth analyzing the behaviours of temperature distributions in the entire structure. The comparison of temperature rise in the steady state obtained in the case of FK and modified space and time GL FK models have been presented in Figures 11 - 12.

As it is visible, for the steady state the temperature distributions, derived by

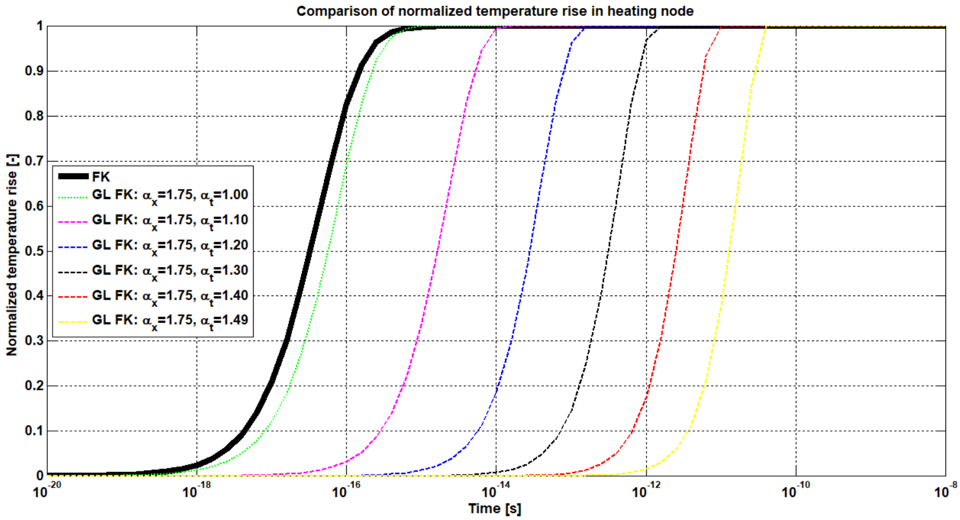

Fig. 9. Comparison of normalized temperature rises in heating node obtained using modified space and time GL FK models for temperature space derivative order equal to 1.75 and different orders of temperature time derivative

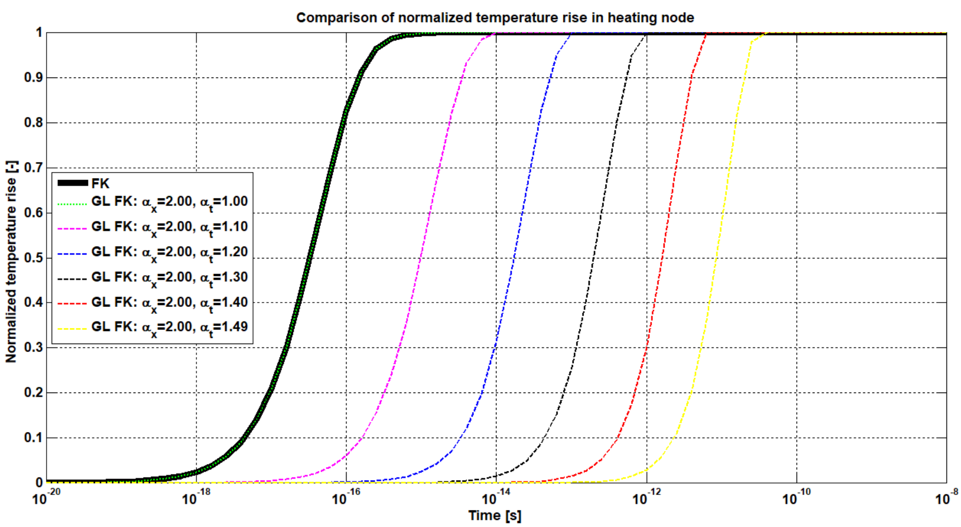

Fig. 10. Comparison of normalized temperature rises in heating node obtained using modified space and time GL FK models for temperature space derivative order equal to 2.00 and different orders of temperature time derivative

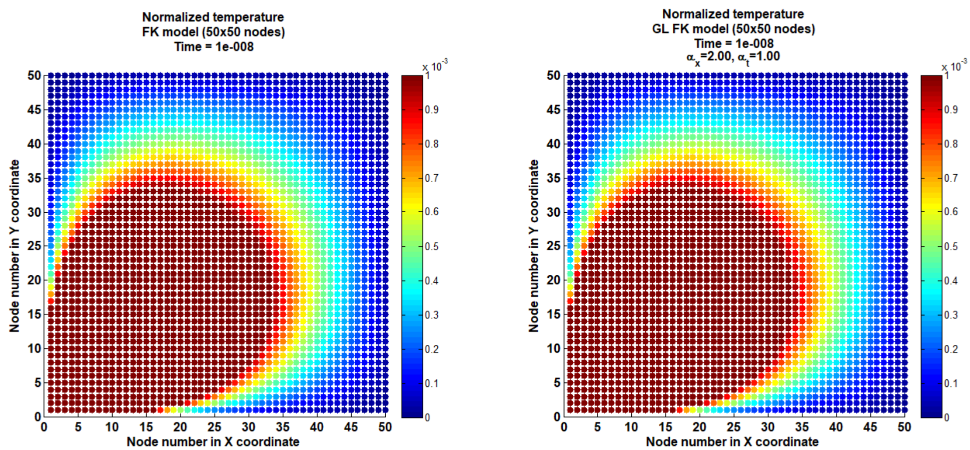

Fig. 11. Comparison of normalized steady state temperature rises in entire structure for FK and modified space and time GL FK models in the case of $\alpha_x = 2$ and $\alpha_t = 1$

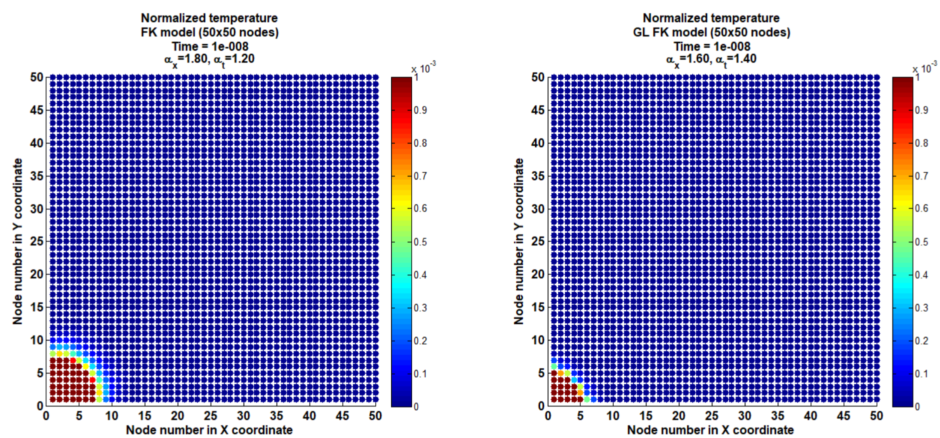

Fig. 12. Comparison of normalized steady state temperature rises in entire structure for modified space and time GL FK models for chosen values of α_x and α_t parameters

the FK model and modified space and time GL FK one for α_x and α_t, are exactly the same, what confirms the previous observations. Of course, it is correct from the physical point of view, because for modified space and time GL FK model reduces to the classical FK one for α_x and α_t. However, the steady state temperature rise in entire structure is different for other pairs of α_x and α_t, what is presented in Figure 12. It means that the modified space and time GL FK model can be used for the heating nodes and it should not be applied in the case of the remaining part of the structure.

Therefore, it can be stated that making some changes of the values of α_x and α_t parameters, the DPL model for certain pair of τ_q and τ_T can be approximated in the heating node. To prove this statement, the fitting procedure of modified space and time GL FK curves to the DPL ones has been carried out. The fitting results are demonstrated in 13. As it can be seen, dark lines present the DPL approaches for chosen pairs of τ_q and τ_T parameters, while the colorful lines present the respective modified space and time GL FK outputs. It is clearly visible that the approximation of the DPL model using the modified space and time GL FK one is possible in the heating node. Moreover, the accuracy of this fitting is at very high level.

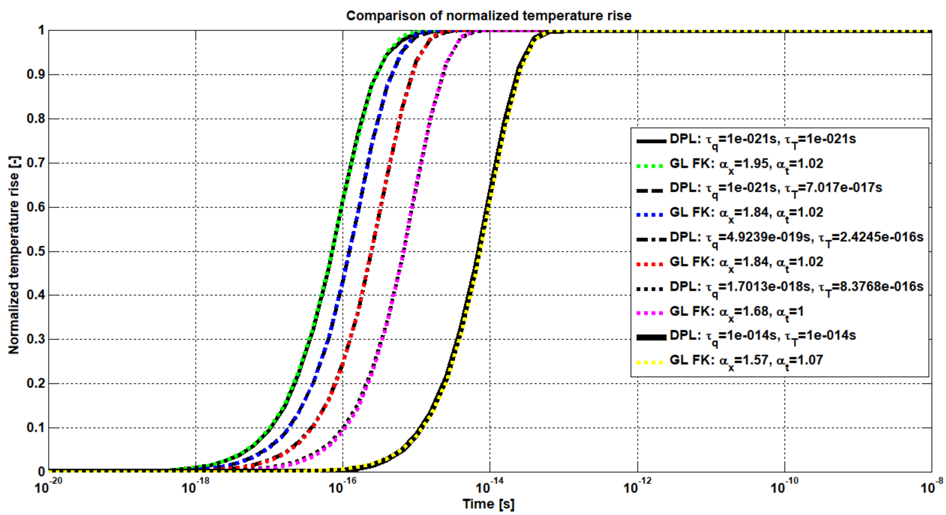

Fig. 13. Comparison of temperature rise in heating node for DPL model for chosen τ_q and τ_t parameters and fitted modified space and time GL FK model for found α_x and α_t values

Then, the equations presented the dependence between the space and time derivative orders and τ_q and τ_T parameters have been determined and presented below.

$$\alpha_x = a_x \cdot \tau_T^{b_x} + c_x \tag{8}$$

$$\alpha_t = a_t \cdot \tau_T^{b_t} + c_t \tag{9}$$

where:

$$a_x = -2.214E65 \cdot \tau_q^{3.3565} \tag{10}$$

$$b_x = 2.854 \cdot \tau q^{0.05437} \tag{11}$$

$$c_x = -3.18E5 \cdot \tau_q^{0.3671} + 1.977 \tag{12}$$

The coefficient of determination of parameters fitting of a_x coefficient, represented by formula 10, is equal to 0.7069, while for the b_x and c_x coefficients, represented by equations 11 and 12, the coefficient of determination is equal to 0.7947 and 0.8586, respectively, what confirms relatively good fitting.

On the other hand, model parameters of α_t value can be derived as follows:

$$a_t = -1.424E10 \cdot \tau_q^{0.4223} + 1540 \tag{13}$$

$$b_t = -6.941E5 \cdot \tau q^{0.4223} + 0.3216 \tag{14}$$

$$c_t = -1.301E5\tau_q^{0.4213} + 1.02 \tag{15}$$

Coefficient of determination values are equal to 0.8567, 0.7299 and 0.7336 for a_t, b_t and c_t expressions, respectively.

The above formulas allow obtaining very good approximation of the DPL model for the entire period of the thermal analysis in the heating. It is also known that it is not possible to approximate the DPL model by the modified space and time GL FK one in the entire structure in the steady state. Thus, it is also worth analyzing the transient analysis of temperature rises obtained using the modified space and time GL FK model. The comparison of the temperature distributions obtained in the entire structure for DPL and respective modified space and time GL FK model, which parameters α_x and α_t have been calculated according to formulas 8 - 15, are presented in Figures 14 - 16.

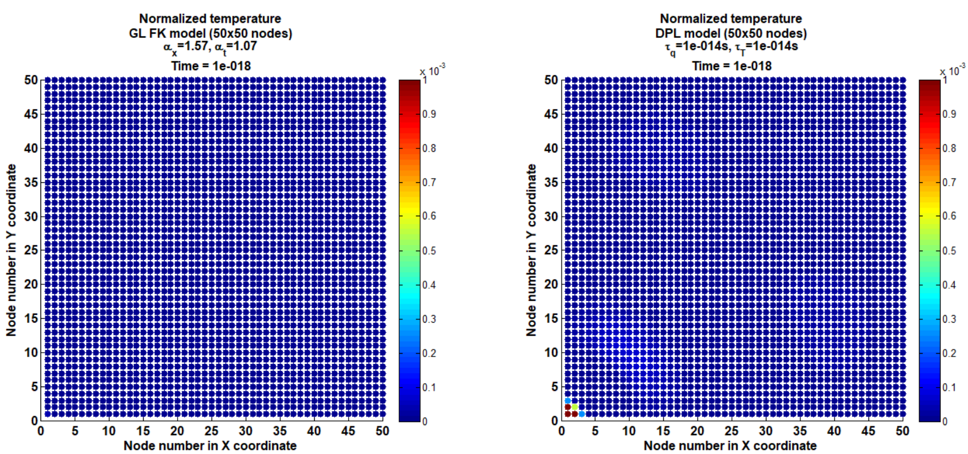

Fig. 14. Comparison of temperature distributions in entire structure in the case of modified space and time GL FK and DPL models in initial part of the thermal simulations

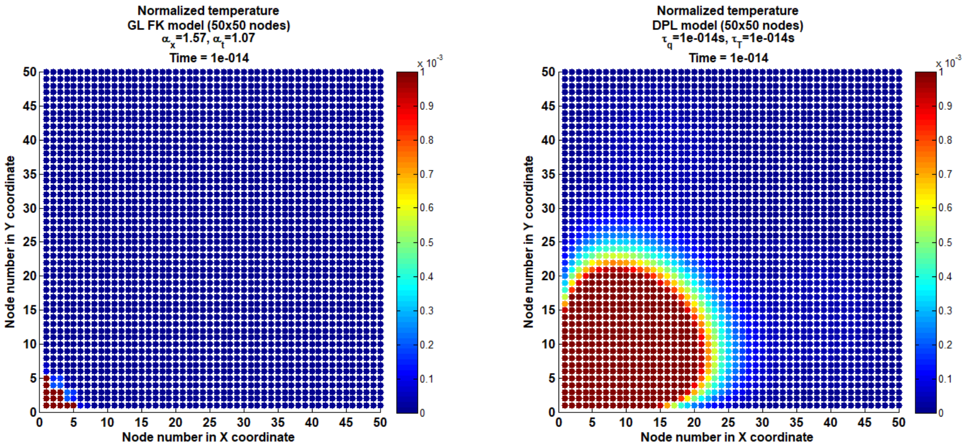

Fig. 15. Comparison of temperature distributions in entire structure in the case of modified space and time GL FK and DPL models in the middle part of DPL temperature rise

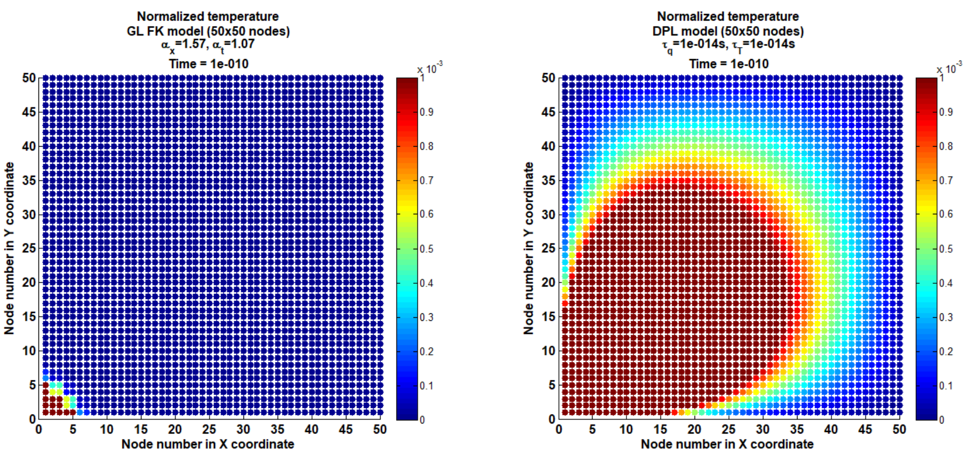

Fig. 16. Comparison of temperature distributions in entire structure in the case of modified space and time GL FK and DPL models in final part of the thermal simulations

As it is clearly visible, the temperature distributions for both DPL and its respective modified space and time GL FK model coincide only in the heating node while for the remaining part of the structure obtained temperature distributions do not agree. Thus, the effective usage of the approximation of the DPL model by the modified space and time GL FK model is possible only for the heating node.

4. Conclusions

This paper includes considerations related to the determination of the approximation scheme of Dual-Phase-Lag model. The approximation method uses the Fourier-Kirchhoff model but the temperature time derivative as well as the space Laplace operator of the temperature function if the FK formula have been replaced by their fractional derivative equivalents based on the Grünwald-Letnikov definition.

In order to obtain the answer if such approximation is possible, the comparison of temperature distributions in investigated rectangular slab, obtained for both the classical Fourier-Kirchhoff and modified space and time GL FK models, has been prepared. Firstly, the analyses focus on the determination of proper order values of the space and time derivatives. Due to this fact, different values of these parameters have been tested. Primarily, the value of the space derivative order was smaller than 2. Then, investigation was based on the case when the space derivative order was equal to 2. Next, the space parameter was established as higher than 2. In all cases the value of the time order derivative has been changed. It occurred that the most reliable results have been obtained for space derivative order from interval $[1.56; 2.00]$ and for value of the time derivative order belonging to the interval $[1.00; 1.49]$.

Moreover, it was also occurred that for time derivatives order greater than 1, the compensation of the temperature rise is needed due to observed decreases under the maximal temperature in the final part of the thermal analyses. After proposed compensation, the obtained temperature rises have the similar characters to the FK and DPL ones. Then, two series of simulations have been prepared. The first one was related to DPL temperature distributions for different pairs of the heat flux and the temperature time lag values. The second one contained the temperature distributions obtained using the modified space and time GL FK model for different values of space and time derivative orders. Received outputs have been compared and for each pair of DPL time lags the respective pair of space and time derivative orders have been found.

Then, the formulas combining the space as well as time derivative orders and the heat flux and temperature time lag values have been determined, what confirmed the possibility of the approximation of DPL model by the modified space and time GL FK one in the heating node. The accuracy of determined approximation scheme is at very high level, what is confirmed by the relatively high value of the coefficient of determination and relatively small values of sum of squared errors and the root-mean-square error.

Furthermore, as it was shown, the approximation of the DPL model using the modified space and time GL FK model is possible only in the case of the heating node. The remaining part of the structure has to be estimated using other techniques.

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WPŁYW ZASTOSOWANIA DEFINICJI POCHODNEJ TEMPERATURY GRÜNWALDA-LETNIKOVA W CZASIE I W PRZESTRZENI NA ROZKŁAD CIEPŁA

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

W pracy wykorzystano nowy model termiczny o nazwie Dual-Phase-Lag. Model ten jest odpowiedni dla struktur nanometrycznych, które obecnie są coraz bardziej. Jednakże, podczas numerycznej impementacji tego modelu mogą pojawić się pewne problemy numeryczne, zaś czas symulacji może być znacznie wydłużony w stosunku do zastosowania klasycznego modelu przepływu ciepła Fouriera-Kirchhoffa. Z tego powodu, rozważania przedstawione w pracy dotyczą wyznaczenia schematu aproksymacyjnego modelu Dual-Phase-Lag opartego na zastosowaniu definicji pochodnej temperatury Grünvalda-Letnikowa, jednocześnie w czasie i w przestrzeni.

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