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Dedicated to the memory of
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TEMPERATURE DISTRIBUTION CHANGES ANALYSIS BASED ON GRÜNWALD-LETNIKOV SPACE DERIVATIVE

Summary

In this paper, the numerical approximation of the Dual-Phase-Lag (DPL) model has been presented. The approximation scheme is based on the Grünwald-Letnikov (GL) definition of fractional derivatives. Moreover, that definition has been applied to the space derivative of the temperature in Fourier-Kirchhoff (FK) model. Then, the Dual-Phase-Lag model has been approximated based on the prepared modification of FK model, which has been called the space GL FK model. Furthermore, the finite difference method methodology for the approximation of the considered thermal model has also been employed. All mathematical formulas obtained during the determination of the approximation scheme are presented in the paper. Numerical examples of temperature distributions obtained in the case of new space GL FK model are also included in the paper. Moreover, the behavior of the model based on order parameter values has also been investigated.

Keywords and phrases: Dual-Phase-Lag model, approximation, Grünwald-Letnikov, fractional derivatives, temperature distribution, numerical computation

1. Introduction

Nowadays, totally new idea of usage of the electronic devices is observed. The societies can use very modern equipment which definitely improve the quality of their life. However, construction and designing of the newest devices cause that new problems appear. Moreover, these problems have to be carefully, but significantly quick resolved. The proper and efficient work of these appliances is very crucial and can decide about their popularity. Currently designed devices are characterized by their very small sizes. It is a big advantage because they can be easily transported and impelmented. Moreover, one small appliance may contain several different functionalities. However, one of the main problems in such equipment is related to the temperature. Due to the small size of these equipments, the internally generated temperatures are very high. Thus, some problems may often occur during their daily usage. Furthermore, thermal problems can even cause serious damages, failures and brokens. Taking into account the thermal issues and physical phenomena, which are observed in such small devices, researchers try to implement new solutions during the planning process and solving described problems.

1.1. Classial and modern heat transfer

The most frequently used thermal model applied during the designing process of electronic structures is Fourier-Kirchhoff one [1] expressed by the following equation:

$$c_v \frac{\partial T(x,y,t)}{\partial t} = -\nabla \cdot q(x,y,t) + q_{gen}(x,y,t) \tag{1}$$

This approach has been successfully employed for two centuries. However, this model is currently insufficient [2], mainly due to the fact that it does not take into consideration physical phenomena which are observed for nanometric structures [3]. Researchers have been prepared different relatively new thermal approaches which can be appropriate for nanometric problems.

On the contrary, new models can be significantly more complex and their numerical implementation may be problematic. Due to this fact, there is a need to propose some approximations of the modern thermal models which also assure highly reliable results during the thermal simulations. One of them is the Dual-Phase-Lag model proposed by Tzou [4]. Its mathematical form can be presented as follows:

$$\begin{cases} c_v \frac{\partial T(x,y,t)}{\partial t} = -q(x,y,t) \\ q(x,y,t) + \tau_q \frac{\partial q(x,y,t)}{\partial t} = -k\nabla T(x,y,t) - k\tau_T \frac{\partial \nabla T(x,y,t)}{\partial t} \end{cases} \tag{2}$$

It can be observed that Dual-Phase-Lag contains two time lags related to the heat flux (τ_q) and the temperature (τ_T). As it was mentioned, this model is appropriate in the case of obtaining the temperature distribution in nanometric electronic structures. However, its numerical implementation, especially in the case of huge discretization meshes can lead to some difficulties. First of all, the big complexity of computation appears, what causes significantly longer time of simulation. Thus, it is needed to approximate the Dual-Phase-Lag model based on approaches which are easier to implement and, at the same time, produce the accurate temperature distributions.

1.2. DPL model approximation

To determine the approximation of Dual-Phase-Lag model, the Grünwald-Letnikov derivative of the space variable formula has been used. It is presented in equation below [6]:

$$D_{0,x}^{\alpha}u(x) = \sum_{k=0}^{m-1} \frac{u^{(k)}(0)x^{-\alpha+k}}{\Gamma(-\alpha+k+1)} + \frac{1}{m-\alpha}\int_0^x (x-\tau)^{m-\alpha-1}u^{(m)}(\tau)d\tau \qquad (3)$$

As it was mentioned previously, the Grünwald-Letnikov definition has been applied to the space derivative. Then, the model has been discretized. Moreover, the central difference has been emloyed. The obtained expression can be described by following equation [6]:

$$D_{0,x}^{\alpha}u(x)_{GL} = \lim_{\Delta x \to 0} \frac{1}{\Delta x^{\alpha}} \sum_{k=0}^{N} (-1)^k \binom{\alpha}{k} u\left(x - k\Delta x + \frac{\alpha \Delta x}{2}\right) \qquad (4)$$

To ensure the numerical implementation of presented approach, the Finite Difference Method has been applied to equation 4. Moreover, it was assumed that to easier application and better visualization of determined formula, the special Gamma function has been used. The final expression is demonstrated by the equation below:

$$D_{0,x}^{\alpha}u(x)_{GL} = \frac{1}{\Delta x^{\alpha}} \sum_{k=0}^{round(\alpha,0)} (-1)^k \frac{\Gamma(\alpha+1)}{\Gamma(k+1)\Gamma(\alpha-k+1)} u\left(x - k\Delta x + \frac{\alpha \Delta x}{2}\right) \qquad (5)$$

It can be concluded that equation 5 is a significant modification of temperature space derivative in Fourier-Kirchhoff model. Then, it will be used to approximate the Dual-Phase-Lag one.

2. Simulation

During the simulation, the simple homogenous structure made of the silicon has been considered. The visualization of the structure and imposed boundary conditions are shown in Figure 1.

Based on the structure presented above, the normalized temperature distribution has been taken into consideration in some different cases. Firstly, the Grünwald-Letnikov derivative has been applied for the space variable of the temperature in Fourier-Kirchhoff equation instead of the classical definition of temperature space

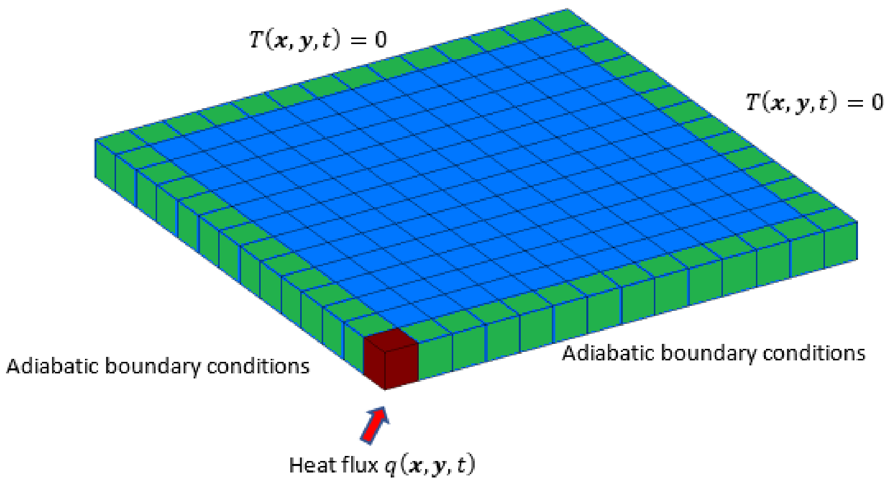

Fig. 1. Structure visualization with imposed boundary conditions

derivative according to the description presented in the previous section. Such modified thermal model, called space GL FK, has been used to obtain the temperature distribution in analyzed structure. The first analyses, presented in Figure 2, is related to the comparison of dynamic behaviors of the temperature rise in heating node received using the space GL FK model for chosen values of the space derivative order α. Moreover, results obtained using classical FK and DPL model, for chosen pairs of the temperature and heat flux time lags, have also been demonstrated.

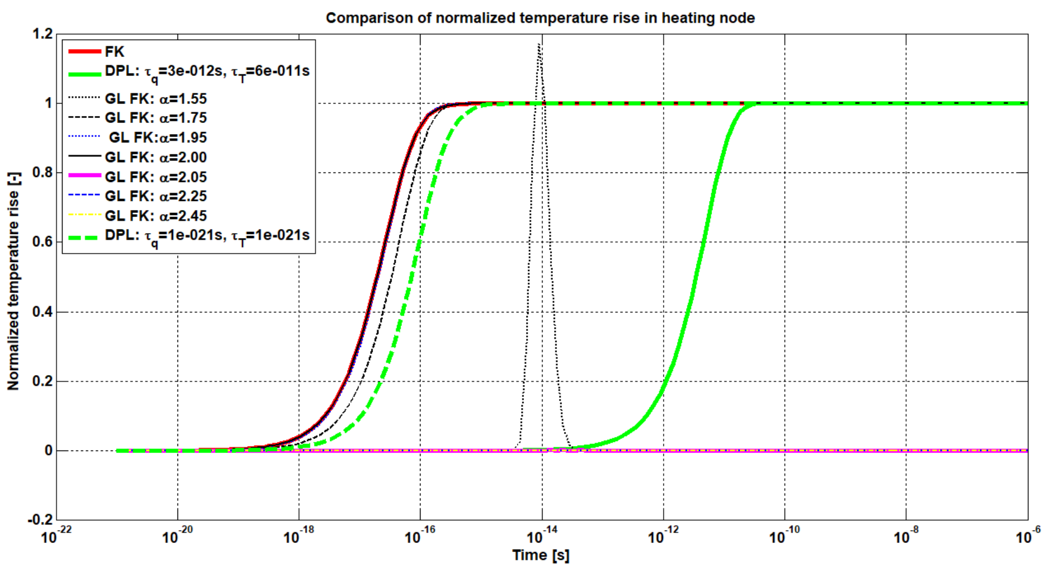

Fig. 2. Comparison of normalized temperature rises in heating node for FK, DPL and space GL FK models

As it can be visible, the temperature rises obtained using DPL models are delayed in relation to the classical FK approach, however behaviors of the temperature rises are similar in the case of both investigated thermal models, what coincides with the previous research [5]. Moreover, the similar situation is also observed for space GL FK model characterized by the parameter α smaller than 2. It is also worth highlighting that the value of the parameter α closer to 2, the dynamic temperature rise behavior more similar to the output of the FK model. It means that for the value of the parameter α tending to 2, the value of the delay of the certain temperature rise, in relation to the FK model, is smaller. Then, when the order α reaches the value of 2, the obtained simulation result coincides exactly with this one yielded using the classical FK approach. Thus, it can be stated that the space GL FK model for the parameter $\alpha = 2$ is equivalent to the classical FK one.

On the other hand, when the value of the temperature space derivative order α is greater than 2, the zero values of the temperature rise have been obtained. It is caused by the form of the space GL FK model and imposed limitations. Moreover, some numerical errors may appear. Due to this fact, matrices inversions cannot be possible and zero values are generated. However, as analyses show, the most important case, from the analytical point of view, is that one regarding the order α smaller than 2 due to its similarity to FK and DPL cases. Additionally, taking into consideration the range, for which the temperature space derivative order α belongs to the interval $[1.5; 2.5)$, values equal or smaller than 2 and equal or greater than 1.5 will be considered in further analyses only.

It is also worth saying that for values of α close to the lower bound of investigated range, numerical errors can also appear. It is visible in Figure 2 for $\alpha = 1.5$ at approximately 0.01 ps. All such cases have been neglected in further analyses.

As it was mentioned previously, for α belonging to the interval $[1.5; 2]$ the dynamic behavior of the temperature rise in heating node is similar to the FK distribution. However, the respective values of temperature rises are delayed in relation to the classical FK model. It means that for some particular cases, the space GL FK model can also be similar to the DPL one. Moreover, the rate of delay depends on the value of parameter α. Values closer to 1.5 cause bigger delays than these ones closer to 2, what is shown in more detail in Figure 3. Apart from that, classical FK and DPL outputs have also been plotted for the reference.

Analysis of this figure suggests the existence of value α belonging to the interval $[1.5; 2]$ for certain pair of temperature and heat flux time lags for the heating node.

However, it is also worth analyzing the temperature distribution not only in the heating node, but also in the entire structure. The sample comparison of the normalized steady state temperature rise in the structure, obtained using the classical FK and DPL model, is demonstrated in Figure 4. Based on the previous research and on the analysis presented in 4, it is known that the steady state heat distributions, for FK and DPL model for each pair of the temperature and heat flux time lags, are exactly the same.

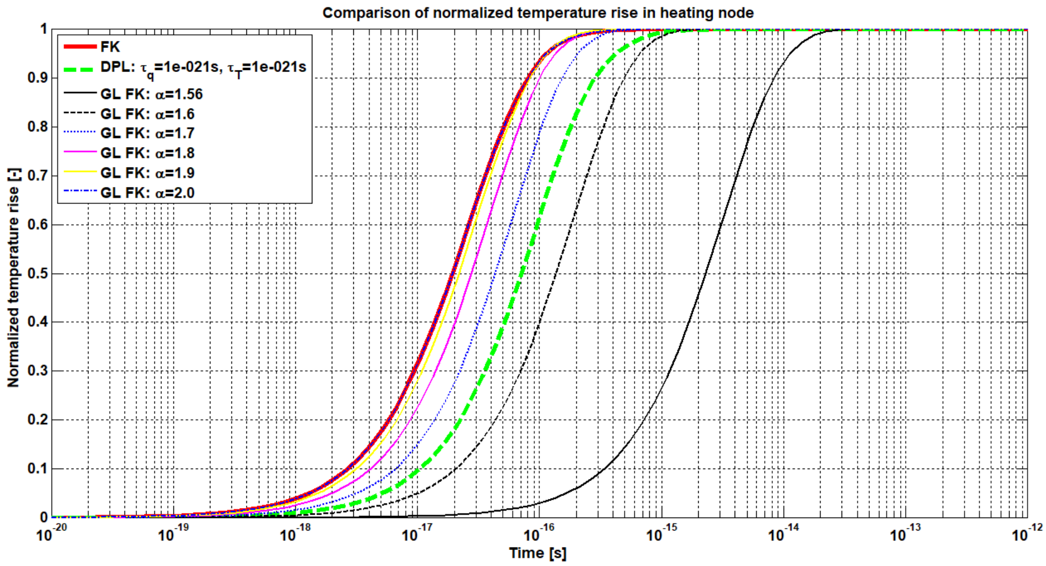

Fig. 3. Comparison of normalized temperature rises in heating node for FK, DPL and space GL FK model for $\alpha \in [1.5, 2]$

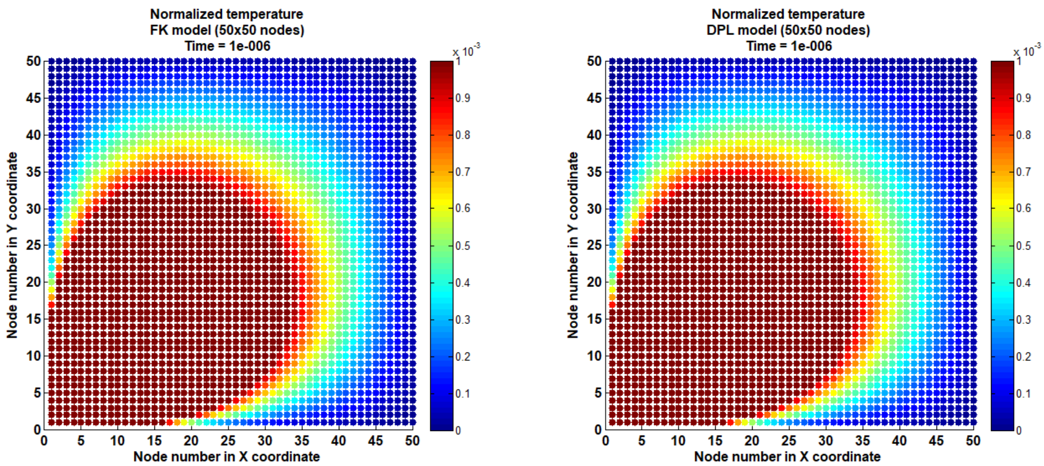

Fig. 4. Comparison of normalized steady state temperature distribution in the structure obtained using FK and DPL models

However, it is also worth considering the steady state temperature distribution in the entire structure for space GL FK models for different values of the temperature space derivative order α. As it is demonstrated in Figure 5, the steady state space GL FK temperature distribution in whole investigated structure differ significantly from these ones obtained using classical FK approach or the DPL one. Obtained normalized temperature rises in most discretization nodes are lower than in FK or DPL cases. However, for $\alpha = 1.7$ the temperature rises are slightly higher than for $\alpha = 1.6$. Thus, an additional analysis has been carried out for bigger values of the α parameter. The results for $\alpha = 1.8$ and $\alpha = 1.9$ have been presented in Figure 6.

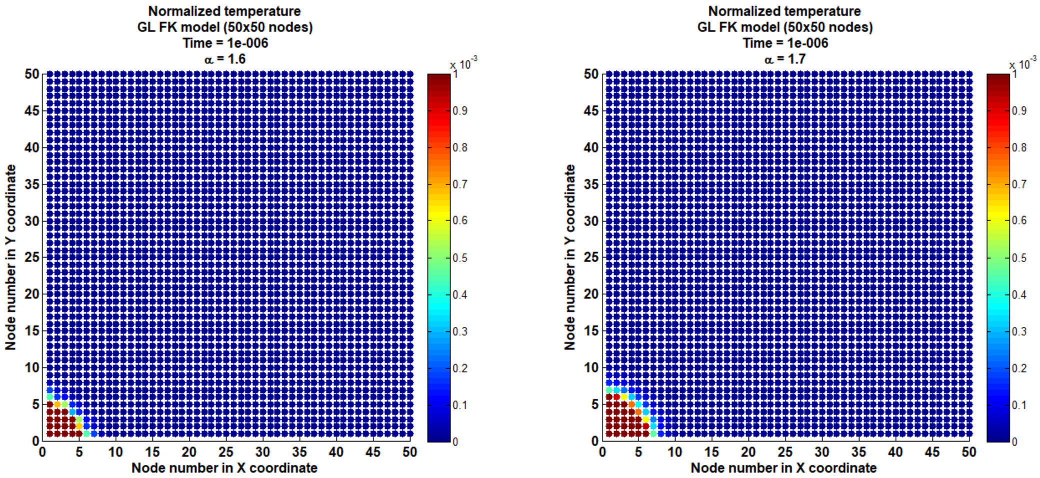

Fig. 5. Comparison of normalized steady state temperature distribution in the structure obtained using space GL FK models for order α belonging to the interval $[1.5; 2]$ part I

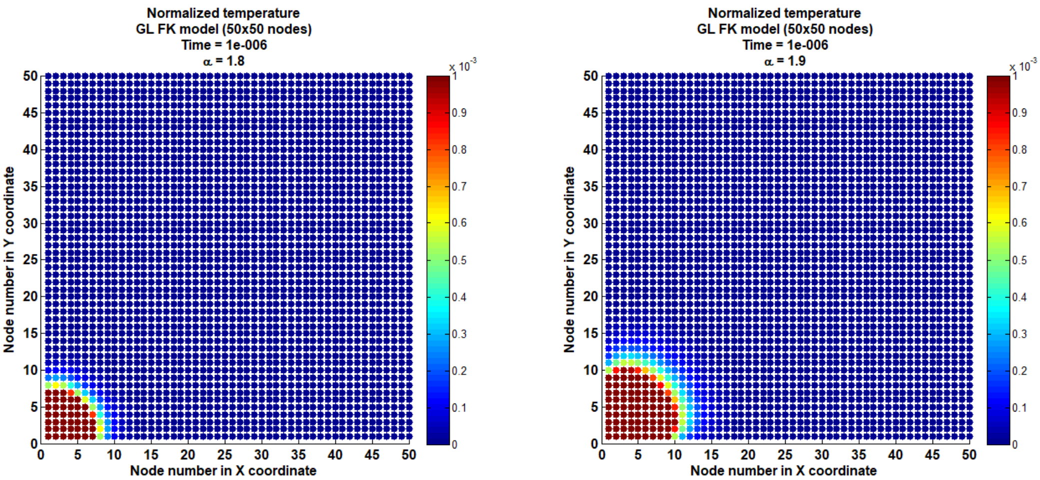

Fig. 6. Comparison of normalized steady state temperature distribution in the structure obtained using space GL FK models for order α belonging to the interval $[1.5; 2]$ part II

As it is noticeable, the normalized steady state temperature distributions are also different from the FK or DPL ones, however the obtained temperature rise values are higher than in the previous cases.

Nevertheless, the steady state temperature distribution in the entire structure for space GL FK cases does not coincide with the FK or DPL approaches as it is observable for the heating node. Thus, it can be stated that the DPL model could be currently successfully approximated by the space GL FK model in heating nodes only. Thus, two series of simulations have been carried out to prove this thesis. Firstly, the temperature distributions for different pairs of the temperature and heat flux time lags have been prepared. It was established that, based on the previously described research, that both time lag DPL parameters should belong to the interval $[1e-21; 1e-15]$. Values smaller than 1e-21 s should cause the significant numerical errors due to the Matlab environment limitations. On the other hand, values greater than 1e-15 may produce results, for which no α values is being found.

Then, the second series of simulations, regarding the normalized dynamic temperature distribution finding based on space GL FK model for α parameter belonging to the interval $[1.5; 2]$, has been carried out. After that, for each pair of DPL parameters, the most proper value of α has been fitted. The fitting procedure has been based on the calculation of the relative error between space GL FK and DPL outputs. The smallest found value of that error indicates the most proper value of the α parameter. The sample comparison of the space GL FK and DPL models results for chosen time lags and found α values is presented in Figure 7.

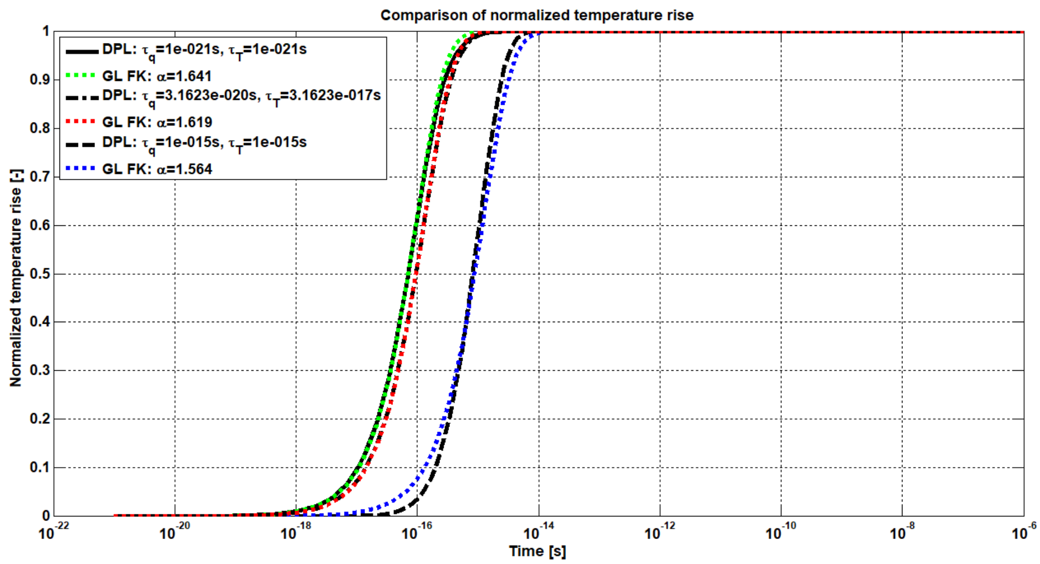

Fig. 7. Comparison of normalized temperature rises in heating node for DPL and respective space GL FK models

As it is visible, the fitting results are characterized by the relatively good compliance with the original DPL outputs. Moreover, the bigger values of the parameter α, the better coincidence of the space GL FK and DPL results.

Based on obtained results, the formula combining the value of the temperature space derivative order α and DPL model parameters values have been derived. Analyses have shown that this dependence can be formulated as the power function according to the following equation:

$$\alpha = a_q \cdot \tau_T^{b_q} + c_q, \tag{6}$$

where coefficients a_q, b_q and c_q can be derived according to the following power formulas:

$$a_q = -2.794e48 \cdot \tau_q^{2.378} \tag{7}$$

$$b_q = 1.215e4 \cdot \tau_q^{0.296} + 0.535 \tag{8}$$

$$c_q = -1.77e6 \cdot \tau_q^{0.4802} + 1.643 \tag{9}$$

The approximations of parameters a_q, b_q and c_q are characterized by the relatively good accuracy. The coefficient of determination for this quantities is equal to 0.941, 0.7293 and 0.9686, respectively. It is also confirmed by the analysis of the sum of quared error (SSE) and root-mean-square error (RMSE) values. For b_q and c_q parameters, they are relatively small. On the other hand, for a_q SSE and RMSE values are significantly bigger, thus the entire approximation scheme for α may generate values, for which the space GL FK outputs do not coincide exactly with approximated DPL ones. Possible erroneous value are the result of the numerical errors generated for extremely small time instant and DPL time lag values. Nevertheless, the proposed approximation reflects the dynamic behavior of the normalized temperature rise in heating with acceptable overall level of accuracy.

In order to check the possibility of applying the proposed approximation to the entire structure, additional analyses have been carried out. The normalized temperature distribution in the structure have been compared for DPL model described by the certain pair of the temperature and heat flux time lags and respective value of the order α. The comparison results are demonstrated in Figures 8 - 10.

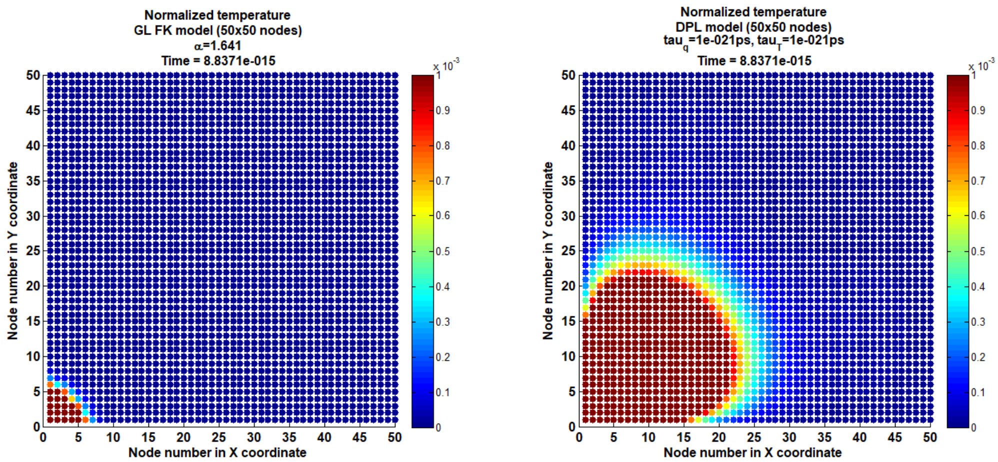

Fig. 8. Comparison of normalized temperature distribution in the structure obtained using DPL and respective space GL FK models during the initial time of DPL model temperature rise

As it is visible, the space GL FK model produces significantly lower temperature values than the DPL one in most structure discretization nodes. Moreover, this situ-

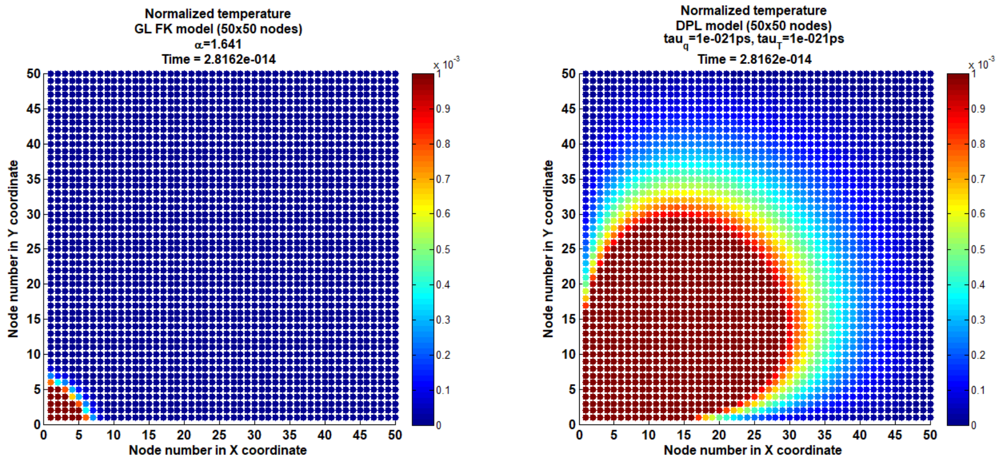

Fig. 9. Comparison of normalized temperature distribution in the structure obtained using DPL and respective space GL FK models during the final part of DPL model temperature rise

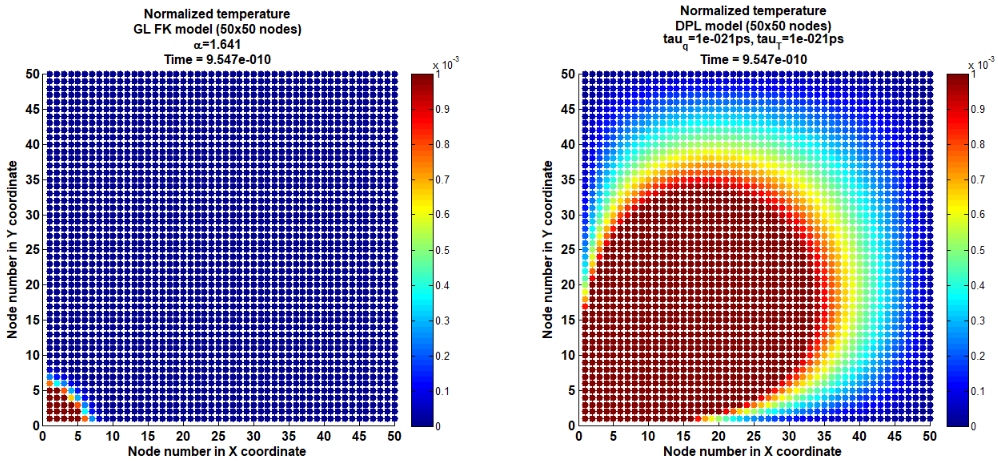

Fig. 10. Comparison of normalized steady state temperature distribution in the structure obtained using DPL and respective space GL FK models

ation is characterized for different time instants. Therefore, the effective DPL model approximation using the space GL FK one is currently possible for the heating nodes only.

3. Conclusions

In the paper, the approximation of DPL model based on the modification of classical FK model, including the Grünwald-Letnikov definition of the temperature space derivative, has been presented. As it occurred, the DPL model can be effectively approximated using the space GL FK model in the case of heating nodes.

The formula combining the space derivative order and both temperature and heat flux time lags has been determined. Prepared analyses confirm relatively good consistence of space GL FK models with the DPL ones in the heating nodes of homogenous materials for some range of space derivative order α and certain pairs of values of τ_T and τ_q values.

However, it occurred that DPL model cannot be approximated by the space GL FK one in the case of temperature distribution determination in the entire structure. The normalized temperature distribution obtained for DPL model differs from this one received using the temperature space GL derivative in FK model.

Thus, in the near future, the common influence of fractional time and space derivatives on the temperature distribution will also considered.

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ANALIZA ZMIAN ROZKŁADU TEMPERATUR W OPARCIU O DEFINICJĘ POCHODNEJ GRÜNVALDA-LETNIKOVA W PRZESTRZENI

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

W pracy zaprezentowano numeryczne przybliżenie modelu Dual-Phase-Lag. Schemat aproksymacyjny bazuje na wykorzystaniu definicji pochodnej temperatury niecałkowitego rzędu Grünvalda-Letnikova. Definicja ta została zastosowana do pochodnej przestrzennej temperatury w klasycznym modelu Fouriera-Kirchhoffa w celu wyznaczenia aproksymacji modelu Dual-Phase-Lag. W celu uzyskania numerycznej postaci rozwiązania, wykorzystano metodę różnic skończonych. Wszystkie otrzymane wzory aproksymacyjne zostały zaprezentowane i dokładnie opisane w niniejszym artykule. Dodatkowo zamieszczono przykłady rozkładu temperatury otrzymane za pomocą nowoskonstruowanego modelu. Wyznaczono ponadto wzór aproksymujący model Dual-Phase-Lag za pomocą zmodyfikowanego modelu Fouriera-Kirchhoffa uwzględniającego zamianę klasycznej pochodnej przestrzennej definicję pochodnej Grünvalda-Letnikova.

Słowa kluczowe: model Dual-Phase-Lag, przybliżenia numeryczne, pochodna niecałkowitego rzędu Grünvalda-Letnikova, rozkład temperatury