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Refining of Numerical Solution for Nonlinear Transient Heat Conduction in a Plate Made of Polymer Composite Material

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Abstract
The object of this paper is the error estimate of the numerical solution for nonlinear transient heat conduction problem for a plate made of a polymer composite material, which is under high-temperature heating. To obtain the refined solution for a given number of time steps for different spatial grids the Romberg method of re-extrapolation was used. It is shown that the process of extrapolation should be monitored by criterion that ensures the results validity.

Keywords: Error estimate, error of solution, transient heat transfer, polymer composite material, parabolic differential equation.

Introduction
Now numerical methods have an enormous spread in many scientific fields using computer simulation techniques. By-turn, the numerical experiment is often used in the study and modeling of the physical processes by solving a wide range of technical issues, since it allows obtaining results of the study, even when to carry out real experiment is difficult. The main criteria of the computer simulation effectiveness is solution accuracy and the computational complexity of the used numerical method. Test problem with the exact solution is used for error estimate of numerical methods. In this case, the accuracy of numerical simulation is characterized by the measure of the numerical result deviation with the exact analytical solution. Heat conduction problems are usually a system of nonlinear differential equations that is why one of the key problem of numerical analysis is to develop a means of monitoring and proof of authenticity of the results, taking into account all known sources of error [1]. Occurrence of an error can be caused by many factors such as lack of fit of analytical and discrete models, round-off error of machine internal representation, etc [5]. The presence of these error components leads to the boundaries uncertainty of the range of the possible values of the total error, and makes difficult its accurate estimate [4]. Therefore, as the numerical characteristic of the results accuracy will be used the estimated probability that the real error is not beyond a certain predetermined level.

Formulation of the Problem
The one-dimensional heat conduction equation for the studied plate made of polymer composite material has the following form

$$\lambda_x(T)\,\frac{\partial^2 T}{\partial x^2}+\frac{\partial \lambda_x(T)}{\partial x}\frac{\partial T}{\partial x}=C_v(T)\,\frac{\partial T}{\partial t}-W(T)\,,$$

where $\lambda_x=\lambda_x(T)$ – integral thermal conductivity of the studied material along X-direction, $C_v=C_v(T)$ – specific heat per unit volume, $W=W(T)$ – source of heat [6] – [9].
Used non iteration implicit scheme for determining the temperature field with heat source when the thermal properties of a material selected from the respective sets of input information against the known temperature distribution in the previous time layer [2], [5]. Thus, the discrete analogue of the differential equation is:

$$\lambda_x\left(T_i^{(n)}\right)\left(\frac{T_{i-1}^{(n+1)}-2T_i^{(n+1)}+T_{i+1}^{(n+1)}}{\Delta x^2}\right)+$$
$$+\frac{\partial\lambda_x(T_i^{(n)})}{\partial x}\,\frac{T_{i+1}^{(n+1)}-T_{i-1}^{(n+1)}}{2\Delta x}=$$
$$=C_v\left(T_i^{(n)}\right)\frac{T_i^{(n+1)}-T_i^{(n)}}{\Delta t}-W\left(T_i^{(n)}\right)$$

where $i=1,2,\ldots,N_x$ – number along X-direction, $n=1,2,\ldots,N_n$ - number of time layer in n-th moment of time t; $(n+1)$ – time layer for time $(t+\Delta t)$, Δx - space step size; Δt – time step size; $\lambda=\lambda(T_i^{(n)})$ - the thermal conductivity of the material for a known temperature $T_i^{(n)}$ in a current time n; $C_v=C_v\left(T_i^{(n)}\right)$ - value of specific heat per unit volume for a known temperature $T_i^{(n)}$ in a current time n; $W=W\left(T_i^{(n)}\right)$ - value of source of heat for a known temperature $T_i^{(n)}$ in a current time n.
To refine the results of the calculation of nonlinear heat conduction problem with a source of heat a modified method was used. The rule of Richardson and Romberg method [2], [3] are used for improve the calculation accuracy without increasing nodes of computational mesh.

Extrapolation by a Known Approximation Order

The following problem must be solved using numerical methods for mathematical modeling of physical processes. Suppose that the first *N*-members are known of a sequence of temperature values $\{T_n\}$. Using this information could whether:

1. to establish that this sequence of temperatures converges to a limit;
2. to find out the limit;
3. to estimate the limit's error;
4. to evaluate the reliability of the error estimation by using some criterion.

This may seem that this problem is not solved at first sight, because too little information. However, in practice, the examples show that in the initial elements of the sequence much more information about the limit of it contains than we think, and due to this, the question is how to find out it.

One way of estimating the error is to compare the calculated value with an extrapolated [3], [5]. Extrapolation is also used to accelerate the convergence of sequences. Known methods for accelerating the convergence based on the fact that the new sequence of temperatures $\{T'_n\}$ is searching by the original sequence of temperatures $\{T_n\}$ and this new sequence tends to the same limit $\lim_{n\to\infty} T'_n = \lim_{n\to\infty} T_n$, but faster.

In some cases, due to the acceleration of convergence is possible to obtain results that could not be obtained within a reasonable time by using other means.

Thus, during the numerical calculation of nonlinear transient heat conduction problem, we got a few members of the sequence of temperatures $T_{n_1}, T_{n_2}, \ldots, T_{n_L}$, whose numbers are not arranged in a row but arbitrarily. Then, we approximately find the limit of the sequence of temperature T by using this data. Then, the temperature difference $T_1 - T$ can be used to estimate the error of an approximate value T_i. However, since the actual value of temperature obtained approximately, so it is necessary to have a criterion to judge the reliability of this estimate (or its accuracy). The set of evaluation criteria and its reliability makes it possible to take a decision about the end of the calculations, in case of if it can be argued that the specified accuracy is reached, or it need to be continued the research.

Consider only those from the variety of extrapolation methods that require knowledge of the numerical values of temperature T_i, rather than through a number i of analytical expressions.

As initial position, we know the results of temperature calculation T_n by the nodes quantity n built of the finite-difference mesh of used numerical method that has k-th of accuracy order (or approximation order), which can be represented as

$$T_n = T + c_1 n^{-k} + \delta(n), \tag{1}$$

where T - exact value; T_n - approximate result approximate result obtained when the quantity of nodes (or when quantity of sum terms), equal to n; c_1 - coefficient that is supposed to be independent of n; k - the order of a method accuracy; $\delta(n)$ - value assumed to be small compared to $c_1 n^{-k}$ when those values n were used in these specific calculations.

In this case, we obtain a single equation with two indeterminates c_1 and T when casting out $\delta(n)$ in (1). To get the second equation we use another well-known member of the sequence of temperatures T_{n_1}. Let $n_1 = n/Q \quad (Q > 0)$ then we come to a system of two equations

$$\begin{cases} T_n = T + c_1 n^{-k}, \\ T_{n/Q} = T + c_1 \left(\dfrac{n}{Q}\right)^{-k}. \end{cases} \tag{2}$$

Subtracting the first equation from the second, we find out that

$$T_{n/Q} - T_n = c_1 n^{-k} \left(Q^k - 1\right),$$

where from it is easy to find out c_1, and thus the temperature T:

$$T = T_n + \frac{T_n - T_{n/Q}}{Q^k - 1}. \tag{3}$$

Using (3) is determined the extrapolated value of the sought temperature $T = T^*$ (according to the rule of Richardson), and owing to using it an approximate value T_n of error estimate $T_n - T^*$ is found. This method of error estimation is called rule Runge.

To construct a more detailed mathematical model of the error we find out the further indeterminates $T, c_1, \ldots, c_L$ by the method of Romberg, using at given $L+1$ the temperature value T_i and representing the problem as a system of linear equations with neglecting small quantities. Then the system of equations is solved by constructing the Lagrange interpolation polynomial [1] L-th power and extrapolating it to $n \to \infty$. Then, in general, a mathematical model error is represented as

$$T_n = T + c_1 n^{-k_1} + c_2 n^{-k_2} + \ldots + c_L n^{-k_L} + \delta(n), \tag{4}$$

where $k_1, \ldots, k_L$ - arbitrary real numbers.

Quality Criterion of Error Estimation

The question arises of the admissibility of the dropping $\delta(n)$ when using the method Romberg for error estimation.

What kind of criteria can apply for it? If the error estimation Δ_n^* of error estimates $\Delta_n = c n^{-k}$ can be found, then the module of the ratio of these assessments should be much less than unity

$$\bar{\delta}_n = \left|\frac{\Delta_n^*}{\Delta_n}\right| << 1. \tag{5}$$

This means that the relative fuzziness of estimation Δ_n is low, and this estimation could be trusted. If $\bar{\delta}_n > 0.3 - 0.5$, then the width of the fuzziness range is comparable with Δ_n, and this estimation should be rejected.

Since the value Δ_n is obtained in the form of a temperature difference $T_n - T^*$ (where T^* - extrapolated value of

temperature), the error estimate of the value Δ_n is error estimate of extrapolated value T^* (with the opposite sign).
What kind of information can be used for such an estimate? We consider the problem of finding the error estimate in the conditions when only the numerical values of temperatures T_n are known.
We apply the following approach. Let designate an extrapolated temperature value T^* as T_n^* which was obtained using the method Romberg for a particular n. Then, increasing n (in Q, Q^2, etc. and Q^m times), we can get the refined sequence of temperature values T_n. Let represent T^* in the form of (1)

$$T_n^* = T + c_2 n^{-k_2} + \delta_2(n), \qquad (6)$$

and get extrapolated temperature twice $T = T_n^{**}$ by repeating Richardson extrapolation formula (3), (where, instead of T_i we use T_i^*). The difference $\Delta_n^* = T_n^* - T_n^{**}$ is the sought error estimate of extrapolated temperature value T_n^*.
As a result of these actions are obtained the twice extrapolated values of the temperature T_n^{**}, when its error is also estimated by re-(third) extrapolation. If this estimation is small in comparison with Δ_n^*, the extrapolated temperature values T_n^* are used as a refined value with the known error estimate and with measure its fuzziness.
Extrapolation process can be repeated as long as the next ratio of the fuzziness width to the estimation value is not be close to one, or does not exceed one.

Numerical Experiment
The numerical experiment was performed for the benchmark problem. The results of calculations and estimates presented in the form of a graph where the abscissa represents the decimal logarithm of the number of time mesh nodes n, and the vertical axis - logarithms of the absolute values of errors (logarithms are more convenient in terms of demonstrativeness, because it is easily determined the order of errors and of numbers n). In this representation, depending close to linear.
Fig. 1-6 the bottom line corresponds to the calculated values of the temperature, the line above - corresponds to the dependence of error of the results extrapolated once, the next line - twice, and so on. During estimation, the value k_1 equals to two and then with increasing numbers j the k_i value is incremented by one. From Fig. 1-8 it is seen that by re-extrapolating very accurate results are obtained.

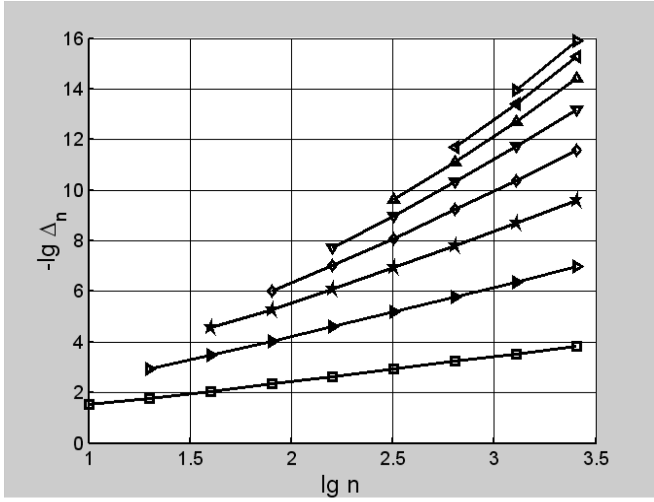

Fig. 1. Results of data extrapolation obtained by doubling the number of items by using the Romberg's method assessed by Runge rule at the number of steps along the X-axis $n_x = 10$ for different time mesh $n_t = 10 \div 5120$, where the abscissa represents the logarithms of time steps number n_t of mesh, and the vertical axis - logarithms of estimates of the absolute values of the relative errors of calculation temperature.

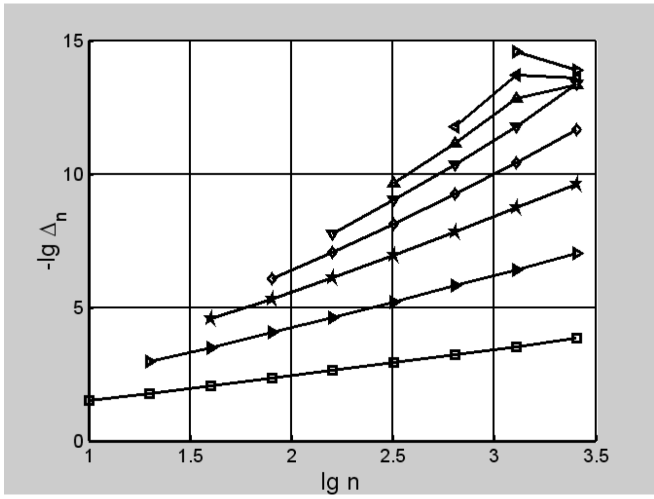

Fig. 2. Results of data extrapolation obtained by doubling the number of items by using the Romberg's method assessed by Runge rule at the number of steps along the X-axis $n_x = 640$ for different time mesh $n_t = 10 \div 5120$, where the abscissa represents the logarithms of time steps number n_t of mesh, and the vertical axis - logarithms of estimates of the absolute values of the relative errors of calculation temperature.

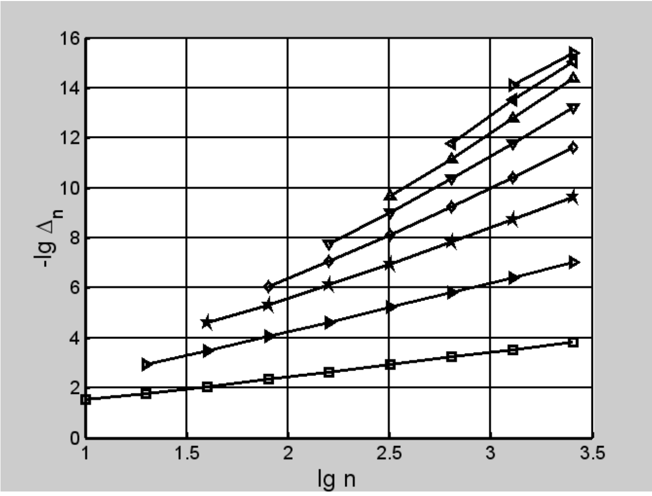

Fig. 3. Results of data extrapolation obtained by doubling the number of items by using the Romberg's method when compared with reference standards at the number of steps along the X-axis $n_x = 10$ for different time mesh $n_t = 10 \div 5120$, where the abscissa represents the logarithms of time steps number n_t of mesh, and the vertical axis - logarithms of estimates of the absolute values of the relative errors of calculation temperature.

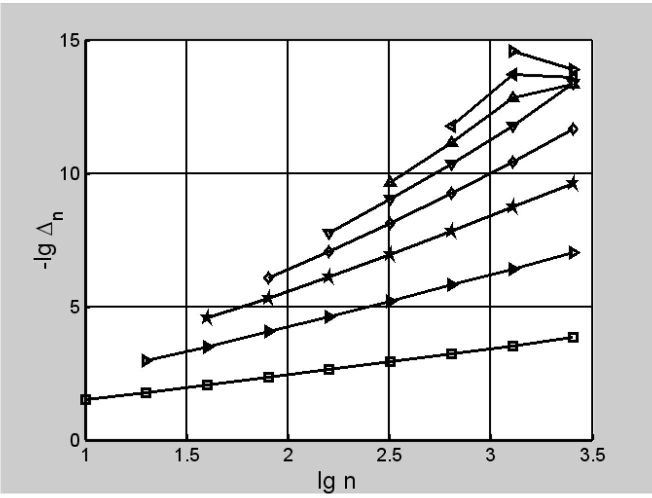

Fig. 4. Results of data extrapolation obtained by doubling the number of items by using the Romberg's method when compared with reference standards at the number of steps along the X-axis $n_x = 640$ for different time mesh $n_t = 10 \div 5120$, where the abscissa represents the logarithms of time steps number n_t of mesh, and the vertical axis - logarithms of estimates of the absolute values of the relative errors of calculation temperature.

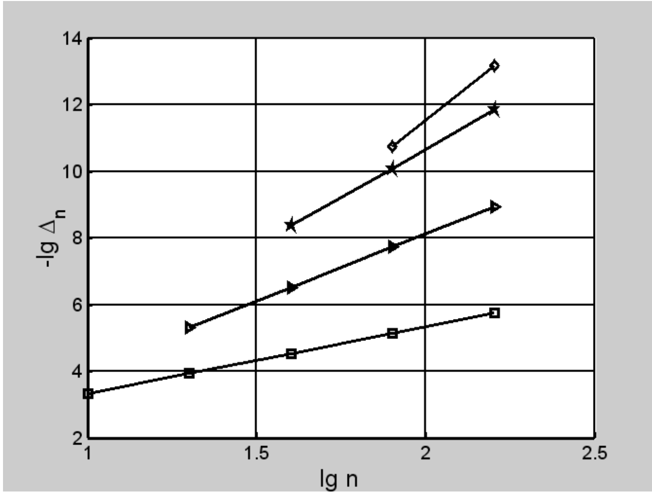

Fig. 5. Results of data extrapolation obtained by doubling the number of items by using the Romberg's method assessed by Runge rule at the number of time steps $n_t = 10$ for different spatial mesh $n_x = 10 \div 160$, where the abscissa represents the logarithms of steps number n_x of spatial mesh, and the vertical axis - logarithms of estimates of the absolute values of the relative errors of calculation temperature.

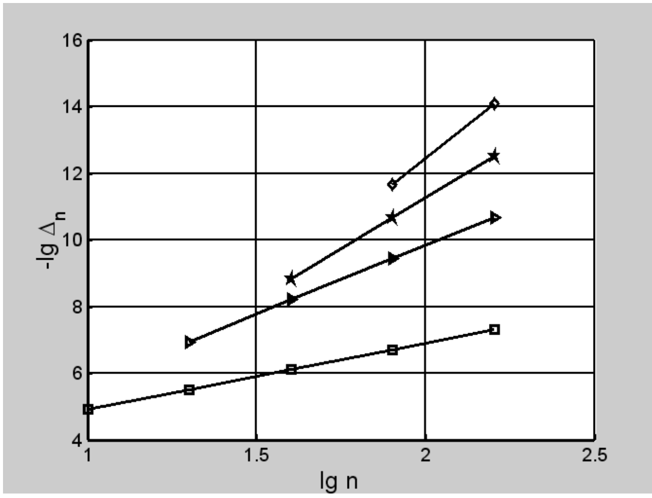

Fig. 6. Results of data extrapolation obtained by doubling the number of items by using the Romberg's method assessed by Runge rule at the number of time steps $n_t = 160$ for different spatial mesh $n_x = 10 \div 160$, where the abscissa represents the logarithms of steps number n_x of spatial mesh, and the vertical axis - logarithms of estimates of the absolute values of the relative errors of calculation temperature.

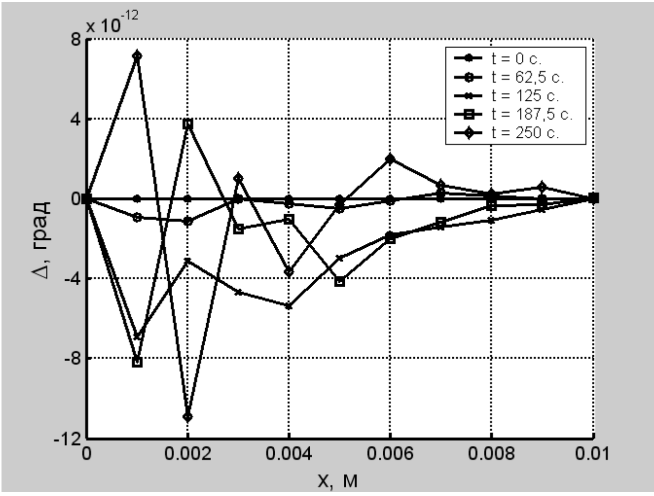

Fig.7. Diagram of the absolute error of refined temperature calculation by using of Romberg's method ΔT, ^{o}C throughout plate thickness along the axis X, m of the mesh size, $Nx = 11$, $Nt = 5121$, where Nx - the number of nodes of the mesh along the X-axis, Nt - the number of nodes of the temporary mesh.

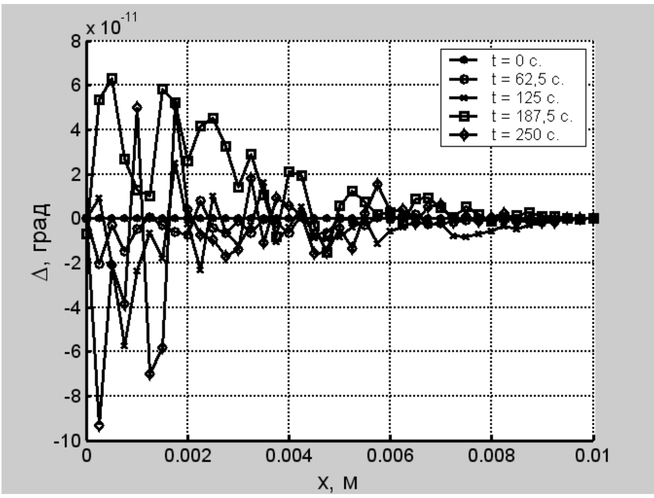

Fig.8. Diagram of the absolute error of refined temperature calculation by using of Romberg's method ΔT, ^{o}C throughout plate thickness along the axis X, m of the mesh size $Nx = 41$, $Nt = 5121$, where Nx - the number of nodes of the mesh along the X-axis, Nt - the number of nodes of the temporary mesh.

Conclusion

This method suggested for getting the more accurate numerical solution of the nonlinear heat conduction problems by methods of extrapolation. Here shown that the application of the methods caused by both form of analyzed sequences and by numerical order of the sequence, which are taking in consideration. Re-extrapolation can significantly improve the results even for slowly convergent sequences, but the process is essentially limited to round-off errors. In this paper shown that the process of extrapolation should be monitored by criterion, which allows you to perform in a way to guarantee the validity of the results.

Thus, the error estimates are obtained in two ways: by comparing with the known analytic solution and without it - through multiple extrapolation and through comparison with the most accurate value. The comparison showed the oneness of the two ratings. It follows that if the exact value of the unknown quantity is unknown (and this in practical calculations so indeed), then for comparing the precision can be used in tables and graphs where instead of accurate can be used the most accurate extrapolated value obtained in the last stage.

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