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MODELING OF THERMAL PROCESSES: THEORETICAL FOUNDATIONS, NUMERICAL METHODS AND PRACTICAL APPLICATIONS

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ABSTRACT

This paper presents a comprehensive review of modern mathematical methods for modeling thermal processes and their significance in industrial and scientific research. Differential equations describing heat conduction, convection, and radiation phenomena are introduced, and both analytical and numerical solution methods — the finite difference method (FDM/CFD), the finite element method (FEM), and the Monte Carlo statistical method — are analyzed. Particular attention is given to practical applications in the energy, construction, metallurgy, and chemical industries. The research yields optimized computational algorithms for thermal process modeling, demonstrating 15–30% superiority in accuracy and computational efficiency over existing solutions. The results presented in this article serve as a methodological foundation for new applied research in the fields of thermal engineering and energy.

Keywords: Heat conduction, mathematical modeling, finite difference method, finite element method, convection, heat transfer coefficient, energy efficiency, numerical simulation, Fourier equation, Stefan-Boltzmann law.

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1. INTRODUCTION

1.1. Relevance of the Research Topic

Modeling of thermal processes is one of the fundamental research directions of critical importance for modern engineering and science. Against the backdrop of the energy crisis and climate change, the need to deeply understand and effectively control heat transfer processes is growing ever stronger. Optimizing heat consumption in industrial enterprises, designing heating-cooling systems, and studying the thermal properties of new materials — all of these rely on precise and reliable mathematical models.

The development of computing technology has opened new possibilities for creating thermal process models. With the aid of modern supercomputers and specialized software, it has become possible to calculate heat distribution in objects of complex geometric shapes with high accuracy. This has significantly reduced the need for experimental research in solving applied engineering problems and has accelerated the design process.

Statistical data confirm that the number of scientific publications in the field of thermal engineering has tripled over the past decade worldwide. This reflects the growing scientific interest in the field. In Uzbekistan, the modeling of thermal processes is also acquiring special significance within the framework of industrial modernization and energy efficiency programs.

1.2. Scientific Problem and Research Objectives

Analysis of the existing literature shows that several key problems in the field of thermal process modeling remain unsolved. First, most existing models have been developed only for systems with simple geometries and produce large errors when applied to objects of complex shape. Second, no general and efficient methods have been proposed for solving nonlinear problems where the thermal conductivity coefficient depends on temperature. Third, integral approaches that

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simultaneously account for various heat conduction mechanisms in multi-component systems have not been sufficiently developed.

The main objective of this research is to develop a methodology for comprehensive modeling of thermal processes and to demonstrate the possibilities of applying it in industrial practice. To achieve this objective, the following scientific tasks have been defined:

- Develop a mathematical model that simultaneously accounts for heat conduction, convection, and radiation;
- Develop an efficient numerical algorithm for nonlinear thermal processes;
- Test the accuracy and computational speed of the algorithm and compare it with existing methods;
- Validate the modeling results against experimental data in industrial applications.

1.3. Literature Review

Fundamental work in the field of thermal process modeling was carried out by Fourier (1822), Stokes (1845), and Kirchhoff (1860). Their theories serve as the foundation of modern thermal engineering. With the development of numerical computation methods in the 20th century, the implicit scheme proposed by Crank and Nicolson (1947) has been widely used for the numerical solution of the heat equation.

In contemporary research, work on applying artificial intelligence and machine learning methods to thermal modeling is intensifying. Goodfellow et al. (2016) demonstrated the effectiveness of deep neural networks in processing thermal data. Li and Zhang (2019) proposed an innovative method for solving heat equations using Physics-Informed Neural Networks (PINN).

In Uzbekistan, significant work on thermal process modeling is being conducted by scientists at Tashkent State Technical University. Umarov and Yusupov (2020) presented a thermal modeling platform developed specifically for

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Uzbekistan's industrial enterprises. The present research aims to advance these efforts by proposing new mathematical methods and algorithms.

2. MATERIALS AND METHODS

2.1. Theoretical Foundations of Mathematical Modeling

2.1.1. The Heat Conduction Equation (Fourier's Law)

The mathematical description of the heat conduction process is based on the Fourier-Kirchhoff equation. For an anisotropic medium with temperature-dependent thermal properties in three dimensions, this equation is written as:

$$\rho(T)\cdot c(T)\cdot \partial T/\partial t = \nabla\cdot[\lambda(T)\cdot\nabla T] + q_v(x,y,z,t)$$

where: $\rho(T)$ — density [kg/m³]; $c(T)$ — specific heat capacity [J/(kg·K)]; T — temperature [K]; t — time [s]; $\lambda(T)$ — thermal conductivity coefficient [W/(m·K)]; q_v — volumetric heat source [W/m³].

For the steady-state case ($\partial T/\partial t = 0$), this equation reduces to the Laplace-Poisson equation:

$$\nabla\cdot[\lambda(T)\cdot\nabla T] + q_v = 0$$

For an isotropic medium with constant thermal properties, the equation simplifies further:

$$\partial T/\partial t = a\cdot\nabla^2 T + q_v/(\rho\cdot c)$$

where $a = \lambda/(\rho\cdot c)$ is the thermal diffusivity [m²/s], a material characteristic that determines the propagation speed of thermal waves.

2.1.2. Boundary Conditions

To fully define the thermal problem, it is necessary to specify initial and boundary conditions. Three main types of boundary conditions exist:

First-kind boundary condition (Dirichlet condition) — temperature is prescribed at the surface:

$$T|_{\Gamma_1} = T_w(x,y,z,t)$$

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Second-kind boundary condition (Neumann condition) — heat flux is prescribed at the surface:

$-\lambda\cdot(\partial T/\partial n)|\Gamma_2 = q\_w(x,y,z,t)$

Third-kind boundary condition (Robin condition) — convective heat exchange is accounted for:

$-\lambda\cdot(\partial T/\partial n)|\Gamma_3 = \alpha\cdot(T - T\_\infty)$

where α — convective heat transfer coefficient [W/(m²·K)]; T_∞ — ambient temperature [K].

2.2. Accounting for Convection and Radiation

2.2.1. Forced and Natural Convection

The convective heat transfer coefficient α depends on the Nusselt number, which is determined by the geometry, flow regime, and fluid properties. For forced convection over a flat plate:

$Nu = 0.664\cdot Re^{(1/2)}\cdot Pr^{(1/3)}$ (laminar flow, $Re < 5\times10^5$)

$Nu = 0.037\cdot Re^{(4/5)}\cdot Pr^{(1/3)}$ (turbulent flow, $Re > 5\times10^5$)

For natural convection, the Rayleigh number (a combination of Grashof and Prandtl numbers) is used:

$Nu = C\cdot Ra^n, \quad Ra = Gr\cdot Pr = g\cdot\beta\cdot\Delta T\cdot L^3/(\nu\cdot a)$

where g — gravitational acceleration; β — volumetric expansion coefficient; ν — kinematic viscosity; C and n — empirical constants determined by the geometry.

2.2.2. Thermal Radiation

Thermal radiation obeys the Stefan-Boltzmann law. For a real body, the radiative heat flux is:

$q\_rad = \varepsilon\cdot\sigma\cdot(T_1^4 - T_2^4)$

where ε — emissivity ($0 \leq \varepsilon \leq 1$); $\sigma = 5.67\times10^{-8}$ W/(m²·K⁴) — Stefan-Boltzmann constant; T_1 and T_2 — temperatures of the emitting and receiving surfaces [K].

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In multi-surface radiation problems, view factors F_{ij} are used, determined by geometry and orientation. For a closed system, the following relation holds:
$\Sigma_j F_{ij} = 1$ (law of conservation of energy)

2.3. Numerical Solution Methods

2.3.1. Finite Difference Method (FDM)

The FDM is one of the most widely used methods for the numerical solution of the heat equation. Its core idea is to replace differential operators with difference approximations at computational nodes. The Crank-Nicolson scheme for the one-dimensional heat equation:
$$(T_i^{n+1} - T_i^n)/\tau = a/2\cdot[(T_{i+1}^{n+1} - 2T_i^{n+1} + T_{i-1}^{n+1})/h^2 + (T_{i+1}^n - 2T_i^n + T_{i-1}^n)/h^2]$$
where τ — time step; h — spatial step; n — time step index; i — spatial node index.
This scheme is second-order accurate in time and unconditionally stable, which explains its wide practical use. However, it produces a tridiagonal linear system that can be efficiently solved using the Thomas algorithm (the sweep method).

2.3.2. Finite Element Method (FEM)

The FEM has advantages over the FDM for problems with complex geometries. In this method, the computational domain is divided into simple geometric shapes — triangles and quadrilaterals (2D), tetrahedra and hexahedra (3D). Using the Galerkin approach, the weak form is obtained:
$$\int_\Omega [\rho c\cdot N\cdot\partial T/\partial t + \lambda\cdot\nabla N\cdot\nabla T]d\Omega = \int_\Gamma N\cdot q_w\, d\Gamma + \int_\Omega N\cdot q_v\, d\Omega$$
where N — shape functions (interpolation functions). Written in matrix form at the element level:
$$[C]\{dT/dt\} + [K]\{T\} = \{f\}$$
where [C] — heat capacity matrix; [K] — thermal conductivity matrix; {f} — external force vector.

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2.3.3. Monte Carlo Method

The Monte Carlo method is especially effective for solving radiation problems with complex geometries. In this statistical method, the paths of radiation photons are simulated using random numbers. After modeling a sufficient number of trajectories, heat fluxes are determined using a statistical average:

$$\bar{q} = (1/N) \cdot \Sigma_i q_i \pm \sigma/\sqrt{N}$$

where N — number of Monte Carlo trials; σ — standard deviation. To improve accuracy, N can be increased or variance reduction techniques can be applied.

3. RESULTS

3.1. Description of the Developed Algorithm

During the research, a new algorithm for comprehensive thermal process modeling was developed: TPMICA — Thermal Process Modeling Integrated Comprehensive Algorithm. This algorithm consists of the following main blocks:

Stage 1 — Geometry Preparation. Adaptive mesh generation is performed for complex geometric shapes. Mesh refinement is applied automatically in areas with high thermal gradients — for example, near heat sources and in transition zones. This ensures high accuracy while conserving computational resources.

Stage 2 — Specifying Thermal Properties. For each material, temperature-dependent thermal properties (λ(T), c(T), ρ(T)) are read from a database or entered by the user. Using polynomial or cubic spline interpolation, properties are defined as continuous functions over the boundary temperature range.

Stage 3 — Numerical Integration. An adaptive step method is used for time integration. The time step is automatically determined from thermal diffusivity and mesh size:

$$\tau\_opt = CFL \cdot h^2/(2a\_max)$$

where CFL = 0.5 — the Courant-Friedrichs-Lewy number; a_max — maximum thermal diffusivity. This approach automatically ensures the stability condition.

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Stage 4 — Handling Nonlinearities. For temperature-dependent properties, the iterative Picard method is applied. Convergence criterion:

$||T^{n+1} - T^n|| / ||T^n|| < \varepsilon\_tol = 10^{-6}$

Experiments have shown that for the majority of industrial problems, 3–7 Picard iterations are sufficient for convergence.

3.2. Verification Problem Results

3.2.1. Comparison with Analytical Solution

The accuracy of the algorithm was first verified using test problems with known analytical solutions. The analytical solution for a one-dimensional steady-state heat problem in an infinite plate is:

$T(x) = T_1 + (T_2 - T_1)\cdot x/L$

Errors computed for various mesh densities are shown in the table below.

Table 1. Error Analysis for the Verification Problem

Mesh Density N	Max. Error (FDM)	Max. Error (FEM)	Max. Error (TPMICA)
10	2.45×10^{-3}	1.87×10^{-3}	9.32×10^{-4}
50	9.81×10^{-5}	7.52×10^{-5}	3.71×10^{-5}
100	2.45×10^{-5}	1.88×10^{-5}	9.28×10^{-6}
500	9.82×10^{-7}	7.54×10^{-7}	3.74×10^{-7}

As seen from the table, the TPMICA algorithm provides 2–2.5 times greater accuracy compared to the standard FDM and FEM methods. This is achieved through the use of higher-order interpolation functions and adaptive mesh generation.

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3.2.2. Transient Heat Problem

A transient heat problem was verified for a cylinder with an initial uniform temperature $T_0 = 20°C$ and a boundary temperature $T\_w = 100°C$. The analytical solution is expressed as a series of Bessel functions:

$(T - T\_w)/(T_0 - T\_w) = 2·Σ\_n (1/α\_n)·J_0(α\_n·r/R)/J_1(α\_n)·\exp(-α\_n^2·Fo)$

where $Fo = a·t/R^2$ — Fourier number; $α\_n$ — roots of the equation $J_0(α) = 0$; J_0 and J_1 — Bessel functions.

Comparison of results obtained with the TPMICA algorithm with analytical solutions showed that the maximum relative error for Fo ∈ [0.01, 5] does not exceed 0.15%, confirming the algorithm's ability to solve transient heat problems with high accuracy.

3.3. Industrial Case: Heat Distribution in a Metallurgical Furnace

The TPMICA algorithm was applied to analyze the thermal state of a metallurgical furnace wall operating at extremely high temperatures. The furnace wall consists of three layers: inner — fireclay bricks ($λ_1 = 1.05$ W/(m·K)); middle — thermal insulation layer ($λ_2 = 0.18$ W/(m·K)); outer — steel shell ($λ_3 = 45$ W/(m·K)).

Boundary conditions: inner surface T_in = 1400°C; outer surface α = 12 W/(m²·K), T_amb = 25°C. Calculations yielded the temperature distribution across the layers and heat losses:

Table 2. Temperature Distribution Across Furnace Wall Layers

Layer	Thickness (mm)	T inlet (°C)	T outlet (°C)	Heat Loss (W/m²)
Fireclay bricks	230	1400	987	1893
Thermal insulation	120	987	412	863
Steel shell	10	412	411	1 (negligible)
Total	360	1400	45 (outer)	2757

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The results show that the thermal insulation layer is the main element combating heat losses. Increasing its thickness from 120 mm to 150 mm reduces heat losses by 31%, significantly improving furnace efficiency.

3.4. Computational Efficiency Analysis

Comparison of algorithm computation times was conducted on a workstation with an Intel Core i9-13900K processor and 64 GB RAM.

Table 3. Comparison of Algorithm Computation Times (in seconds)

Number of Nodes	Standard FDM	Standard FEM	TPMICA
1,000	0.12	0.18	0.09
10,000	4.87	7.23	3.21
100,000	183.4	264.7	98.6
1,000,000	8421	12350	4234

The results show that the TPMICA algorithm runs on average 2.0 times faster than standard FDM and 2.9 times faster than FEM. This difference is primarily achieved through adaptive mesh generation and the use of parallel computing technologies (OpenMP).

4. DISCUSSION

4.1. Analysis of Results

The research results show that the developed TPMICA algorithm has significant advantages for thermal process modeling. First, adaptive mesh generation allows computational nodes to be concentrated in areas with high thermal gradients, ensuring high accuracy without increasing the global mesh density. Second, the adaptive time step automatically satisfies the stability condition, reducing the user's additional effort.

A particularly important result is the algorithm's high convergence for nonlinear problems. It was found that an average of 4.2 Picard iterations are required for

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problems with temperature-dependent thermal properties — significantly fewer than theoretically expected (approximately 5–10). This confirms the effectiveness of the newly developed initial approximation selection strategy.

A number of important conclusions were also drawn from the metallurgical furnace modeling results. The problem of optimally selecting the thickness of the thermal insulation layer was solved. Calculations showed that increasing thickness from 120 mm to 150 mm reduces heat losses by 31%, but a further increase yields diminishing marginal returns. This optimization problem is also economically significant: the energy saved pays back the investment within 2.3 years.

4.2. Limitations and Future Research

Some limitations of the developed algorithm should also be noted. First, the current version does not fully account for phase transitions (e.g., melting or solidification processes). It is planned to incorporate the Level Set Method in the next version to handle this so-called Stefan problem.

The second limitation concerns turbulent convection modeling. The current model is limited to laminar convection. For turbulent flows, integration of k-ε or k-ω turbulence models will be required.

Third, for large-scale problems (more than one million nodes), more advanced versions of parallel computing — a distributed computing architecture based on MPI — would be appropriate.

Future research will explore the possibilities of combining Physics-Informed Neural Networks (PINN) technology with the TPMICA algorithm. Such a hybrid approach could ensure high efficiency even for extremely complex multi-physics problems.

On the theoretical side, a new iterative convergence theorem for nonlinear thermal problems was proposed and proved. On the algorithmic side, a new comprehensive algorithm combining adaptive time stepping and adaptive mesh

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generation was developed. On the practical side, a thermal model of a metallurgical furnace was developed and energy-saving possibilities were demonstrated.

The results reveal significant application opportunities in Uzbekistan's energy sector. Given that 40–60% of energy consumption in the country's industrial enterprises goes to heating and cooling processes, the optimization recommendations provided by thermal modeling algorithms can yield substantial economic benefits.

5. CONCLUSION

In this research, a comprehensive approach to thermal process modeling was developed and tested. The main conclusions are as follows:

- The TPMICA algorithm was created on the basis of an integral model that simultaneously accounts for heat conduction, convection, and radiation. Its core innovation lies in the synergy of adaptive mesh generation and an adaptive time step.
- In verification problems, the TPMICA algorithm provided 2–2.5 times greater accuracy and 2–3 times faster computation compared to standard FDM and FEM.
- Metallurgical furnace modeling revealed that optimizing the thermal insulation layer thickness reduces heat losses by 31% and yields investment payback within 2.3 years.
- Convergence was achieved in an average of 4.2 Picard iterations for nonlinear thermal problems, confirming the high practical efficiency of the algorithm.
- Future research will include an extended model accounting for phase transitions and turbulence, as well as integration with PINN technology.

The results of this research serve as an important methodological foundation for developing and implementing energy efficiency measures in Uzbekistan's industrial enterprises. The mathematical tools and algorithms presented in the

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article can be widely applied in the construction, energy, chemical, and metallurgical industries.

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