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SKOB, Yu. O.[1] (https://orcid.org/0000-0003-3224-1709),
KALINICHENKO, M. Yu.[1] (https://orcid.org/0000-0002-8685-065X),
MAMONTOV, I. O.[2] (https://orcid.org/0000-0002-7040-6247),
MAIBORODA, R. I.[3] (https://orcid.org/0000-0002-3461-2959),
RASHKEVICH, N. V.[3] (https://orcid.org/0000-0001-5124-6068),
and OTROSH, Yu. A.[3] (https://orcid.org/0000-0003-0698-2888)

[1] National Aerospace University,
17, Chkalov St., Kharkiv, 61070, Ukraine,
+380 57 707 4080, khai@khai.edu
[2] Kyiv National University of Civil Engineering and Architecture,
31, Povitrianykh Syl Ave, Kyiv, 03037, Ukraine,
+380 44 248 4901, Knuba_admin@ukr.net
[3] National University of Civil Defence of Ukraine,
94, Chernishevska St., Kharkov, 61023, Ukraine,
+380 57 707 3403, nuczu@dsns.gov.ua

MATHEMATICAL MODELING AND NUMERICAL ANALYSIS OF HEAT TRANSFER IN SOLIDS OF COMPLEX SHAPE

Introduction. *Emergency situations may lead to explosions accompanied by the release of heat and pressure waves that destroy structures in their path and cause fires.*

Problem Statement. *Modeling heat transfer in solids of complex geometry remains a critical task, as predicting the distribution of temperature fields is essential in the design of protective structures. Therefore, the development of a new mathematical model that adequately describes transient thermal processes in solids, as well as the creation of an efficient numerical method and its implementation as a modern information system for engineering analysis and prediction, is highly relevant.*

Purpose. *To perform mathematical modeling of unsteady temperature fields in solids within regions of significant temperature gradients arising from accidental explosions of gas mixtures.*

Materials and Methods. *Numerical modeling of transient heat transfer processes in multiply connected solids of complex geometry, surrounded by a thermally conductive gaseous medium, has been carried out using a unified finite-difference algorithm.*

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Results. *A coupled direct problem involving the flow of a continuous gaseous medium, heat transfer between the gas and solid, and heat conduction within the solid has been considered. The mathematical model accounts for the spatial transfer of mass, momentum, and energy, as well as the complex geometry of streamlined solids. The model has been verified through comparison with analytical solutions to benchmark problems involving an infinite steel plate. Three-dimensional temperature fields in spatially complex solids have been obtained for individual geometric primitives and their combinations. Heat transfer simulations have been performed for a turbine blade with a continuous cross-section and internal cooling channels.*

Conclusions. *The newly developed mathematical model has demonstrated suitability for engineering applications in thermal analysis and predictive modeling. The resulting three-dimensional temperature fields can be used to assess the thermal stress state and strength characteristics of structural elements located within the impact zone of high excess pressure caused by accidental explosions of gas mixtures at industrial sites.*

Keywords: numerical modelling, heat transfer, thermal conductivity, solid body of complex shape, isotherms, temperature field.

Emergency releases of flammable and toxic gases at high-risk enterprises lead to the formation of gas-air mixtures that move in the surface layer of the atmosphere under the influence of wind [1] and other environmental factors [2]. The shape of the cloud significantly depends on the source of the emergency release [3]. An explosion of gas-air mixture leads to the generation of a pressure wave, which moves from the epicenter of the explosion, gradually losing its intensity. The blast wave causes shock-pulse loads on the structures of industrial buildings and maintenance personnel. Depending on the magnitude of excess pressure in the shock wave front, destruction [4] and human injury of varying severity are possible [5]. The transition of combustion of a gas mixture from deflagration to detonation mode significantly increases the scale of consequences [6]. The terrain plays a significant role in the distribution of probability fields of destruction and injury [7], as it influences the spread of damaging factors from the source of disturbance of environmental parameters. The same circumstance allows the use of structures such as a wall in the path of a blast wave or thermal radiation to protect personnel and buildings. However, the protective wall is subjected to significant shock and impulse loads, and its material experiences extreme stress. To prevent the wall from collapsing, it is necessary to ensure its sufficient thickness and durable material [8, 9]. In addition, the maximum permissible stresses, based on which the material for manufacturing the protective structure is selected [10], depend on the ambient temperature. The problem is that the temperature state of the surrounding atmosphere during an explosion and fire changes quickly and significantly [11]. A transient thermal load on the environment can lead to unacceptable changes in the strength characteristics of protective structures and excessive temperature stresses in critical sections [12]. For optimal control of such non-stationary modes of the state of the protective infrastructure, it is necessary to have time-dependent three-dimensional temperature fields in its elements. Prediction and analysis of thermal fields using mathematical modelling makes it possible to avoid unacceptable temperature rises or the occurrence of critical temperature changes and take them into account when designing protective structures. In addition, non-stationary heat transfer problems often arise when modelling various processes of atmospheric ecology associated with fires, when surrounding objects are subjected to significant thermal load, under the influence of which they heat up, smoulder, release harmful substances into the atmosphere, etc. It is known that the most reliable data on the state of the structural material of a structure under certain conditions can be obtained through a physical experiment [13]. However, a computational experiment based on adequate mathematical modelling is preferable due to lower costs and the ability to obtain the entire set of necessary information in an engineeringly acceptable time. For example, such computer systems as ANSYS [11] or LIRA [15] make it possible to determine the stress state in a structure and estimate its remaining life resource [14]. While in conditions of an undisturbed environment the main influencing factors will be determined by climatic parameters [2], then in extreme accident conditions [16] large temperature gradients will prevail [17].

The purpose of this work is the numerical modelling of three-dimensional temperature fields in homogeneous multiconnected solids during their heating (cooling) in a gaseous heat-conducting medium. Analytical methods for solving such problems turn out to be effective only for solids of simple shape [18]. In this case, the calculated non-stationary dependences of the temperature field are expressed in the form of exponential series, the convergence of which depends on the location of the control point inside the body and the time since the start of the process. Numerical methods based on modern computer technology make it possible to overcome these shortcomings and solve the problem without the use of complex hierarchical methods, such as step-by-step modelling [19]. A number of works propose a modelling method that is based on the use of the finite-difference method and the finite element method [20], however, as a rule, calculations are carried out without taking into account the multidimensionality of the process [21] or only for infinitely high rates of heat exchange between solids and the environment [22]. As a rule, modern models are not integrated with modules for assessing the risks of structural failure under the influence of changes in thermal loads [23]. Therefore, the creation of a new mathematical model that adequately describes transient thermal processes in solids, the development of an effective method for solving the problem and its implementation in the form of a modern information system that can be used for engineering purposes for analysis and prediction is a pressing issue.

Basic equations of the mathematical model. To describe the processes of motion of a gaseous medium surrounding a solid body, truncated Navier-Stokes equations are used, obtained by discarding viscous terms (Eulerian approximation with source terms) with the assumption that the main influence on the process is exerted by the convective exchange of mass, momentum and energy [24]:

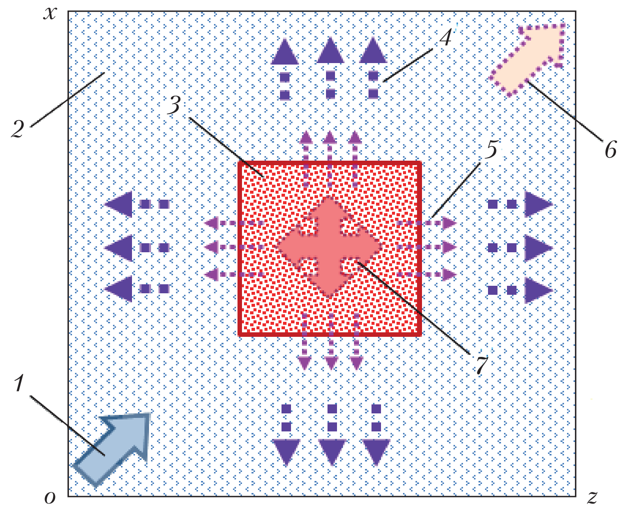

Fig. 1. General calculation scheme of heat transfer: *1* — oncoming gas flow; *2* — ambient gas environment; *3* — solid; *4* — heat flow in gas; *5* — heat transfer from solid to gas; *6* — outlet gas flow; *7* — heat flow in solid

$$\frac{\partial \vec{a}}{\partial t}+\frac{\partial \vec{b}}{\partial x}+\frac{\partial \vec{c}}{\partial y}+\frac{\partial \vec{d}}{\partial z}=\rho \vec{f}, \qquad (1)$$

where $\vec{a} \rightleftarrows \vec{b} \rightleftarrows \vec{c} \rightleftarrows \vec{d} \rightleftarrows \vec{f}$ — vector-columns reflecting the laws of conservation of mass, momentum and energy of air (or gas mixture [7]), ρ — density of air (gas-air mixture).

The calculation area Ω is a parallelepiped with rectilinear forming axes, located in the right Cartesian coordinate system (X, Y, Z) with the base in the XOZ plane (the Y axis is oriented in the direction opposite to the action of the Earth's gravity) (Fig. 1). The calculation area is divided into spatial cells, and the dimensions of the faces are selected from the condition of a sufficiently complete representation of the volume and surfaces of the solid body.

The law of conservation of energy for each calculated "solid" cell (without heat sources) can be presented in integral form:

$$\iiint_v \rho \frac{d(C_v T)}{dt} dV = \iiint_v \operatorname{div}(q) dV, \qquad (2)$$

where V — elementary calculation volume; T — temperature; C_v — heat capacity at a constant volume of solid material; t — time; q — the vector field of the heat flow, which is determined according to Fourier law

$$q = -\lambda g\,\mathrm{rad}T. \quad (3)$$

The law of energy conservation for each calculated "solid" cell (without heat sources) can be.

Let's apply the Ostrogradsky-Gauss theorem to the right-hand side of the equation (2):

$$\iiint_v \mathrm{div}(-\lambda g\,\mathrm{rad}T)\,dV = \iint_\sigma -\lambda g\,\mathrm{rad}T, \vec{n})\,d\sigma, \quad (4)$$

where σ — the surface area bounding a solid volume and having an external normal $\vec{n}(\sigma\vec{n})$.

Boundary conditions. The heat flow at the boundary of a solid cell connected to a gas cell can be determined according to Newton law:

$$q_w = \alpha(T_w - T_e) = -\lambda \frac{\partial t}{\partial n}, \quad (5)$$

where T_w — temperature on the wall; T_e — temperature in the conjugated gas cell; α — heat transfer coefficient.

Assuming the same cell size in all directions, equation (5) can be simplified:

$$\alpha(T_w - T_e) \cong -\lambda \frac{T_w - T_0}{2h}. \quad (6)$$

Having performed a number of identical transformations, we will get the ratio for the temperature on the wall:

$$T_w = \frac{h\alpha T_e + 2\lambda T_0}{h\alpha + 2\lambda}. \quad (7)$$

Thermal diffusivity coefficient for a solid material with heat capacity c_v and density ρ is defined like this:

$$\alpha = \frac{\lambda}{c_v \rho}. \quad (8)$$

Let's use a dimensionless heat transfer parameter Bi for the cell:

$$\overline{Bi} = \frac{\alpha h}{\lambda}. \quad (9)$$

Then the relation (7) can be transformed into a form convenient for calculations:

$$T_w = \frac{T_e \frac{\overline{Bi}}{2} + T_0}{\frac{\overline{Bi}}{2} + 1}. \quad (10)$$

When setting boundary conditions for "gas" faces, it is assumed that the flow component of the velocity does not exceed the speed of sound. Boundary conditions at the inlet are specified on the surfaces of those faces adjacent to the boundaries of the computational domain through which atmospheric air enters the computational domain. The free flow at the entrance to the region is determined by the values of the total enthalpy, the entropy function, the direction of the flow velocity vector, and the relative mass gas density.

The input flow parameters are determined using the relation for the "left" Riemann invariant [25]. In impermeable areas that limit the calculated area of the solid surfaces, the "no-flow" conditions are met. Outlet boundary conditions are specified on the surfaces of those faces of finite-difference cells that are adjacent to the boundaries of the computational domain through which the gas mixture is assumed to flow. In the outlet regions, in addition to atmospheric pressure, relations for the "right" Riemann invariant are used [25].

Initial conditions. At the initial moment of time, environmental parameters are accepted in all "gaseous" cells of the computational domain, and the temperature distribution in the solid is assumed to be uniform over the volume. Under intense influence of the ambient temperature, which corresponds to a heat transfer coefficient equal to infinity, the body surface temperature instantly takes on a value equal to the ambient temperature.

At the initial moment of time, environmental parameters are accepted in all "gaseous" cells of the computational domain. In cells occupied by a cloud of gaseous impurities, which was formed as a result of an instantaneous ejection, the relative mass concentration of the impurity is taken equal to $Q = 1$ (100 %). In cells with evaporation or outflow of gas, the law of change in gas consumption is set.

Numerical solution method. The laws of conservation of mass, momentum, and energy of the surrounding gas in integral form for each calculated gas cell are numerically solved using the arbitrary discontinuity decay scheme (Godunov method [22]), which ensures the construction of discontinuous solutions without identifying discontinuities. The set of gas-dynamic parameters in all cells at a moment of time t^n represents a known solution on the time layer with index n. The parameters at the next time moment $t^{n+1} = t^n + \tau$ are calculated by applying explicit finite-difference approximations. The stability of the finite-difference scheme is ensured by choosing the time step size τ.

For a solid cell with dimensions h_x, h_y and h_z along the coordinate axes, the stability condition for the finite-difference scheme looks like this:

$$2\alpha\tau \le \frac{1}{\dfrac{1}{h_x^2 + \dfrac{1}{h_y^2}} + \dfrac{1}{h_z^2}}. \tag{11}$$

Then the time step for the explicit calculation scheme can be determined from the relation

$$\tau \le \frac{1}{2\alpha\left(\dfrac{1}{h_x^2 + 1/h_y^2} + \dfrac{1}{h_z^2}\right)}. \tag{12}$$

Since the time step for gas cells is an order of magnitude smaller than the step for solid cells, in the case of a stationary or steady heat-conducting gaseous medium surrounding the solid body, it is advisable to "freeze" the gas parameters in time. This allows significantly reducing the time spent on calculations.

Numerical model validation. The adequacy of the developed mathematical model of heat transfer is carried out on the basis of comparison of numerical modelling with known analytical solutions of one-dimensional test problems for an infinite plate with different initial, boundary conditions and variable intensity of heat transfer with a heat-conducting gaseous environment.

Test problem 1. The unsteady process of cooling of an infinite steel plate is considered under the condition of an infinitely high intensity of heat exchange with the surrounding gas.

At the initial moment of time, the temperature in the plate has a constant value

$$T|_{\tau=0} = T_0. \tag{13}$$

At one plate boundary the following condition is satisfied:

$$T|_{x=0} = T_w, \tag{14}$$

and on the other boundary the following condition is satisfied:

$$\left.\frac{\partial T}{\partial x}\right|_{x=h} = 0. \tag{15}$$

The analytical solution for the distribution of the temperature parameter is represented by an infinite series

$$\Theta = \sum_{n=1}^{\infty} A_n \cos[\mu_n(1-\eta)] / \exp(-\mu_n^2 F_0), \tag{16}$$

where the coefficients μ_n and A_n look like this:

$$\mu_n = \frac{(2n-1)\pi}{2}, \tag{17}$$

$$A_n = \frac{(-1)^{n+2} 2}{\mu_n}. \tag{18}$$

The dimensionless arguments of time $F_0 \equiv \alpha\tau/h^2$ (Fourier number) and current coordinate $\eta \equiv x/h$ are use in the calculations.

The results of analytical and numerical solutions comparison is presented in Fig. 2.

Test problem 2. The unsteady process of heat conduction in an infinite plate with a gradient distribution of the initial temperature under the condition of an infinitely high intensity of heat exchange with the surrounding gaseous medium is considered.

At the initial moment of time, the temperature in the plate changes according to the law

$$T|_{\tau=0} = T_w + \Delta T \frac{x}{h}. \tag{19}$$

The following condition is satisfied at both plate boundaries:

$$T|_{x=0} = T|_{x=h} = T_w. \tag{20}$$

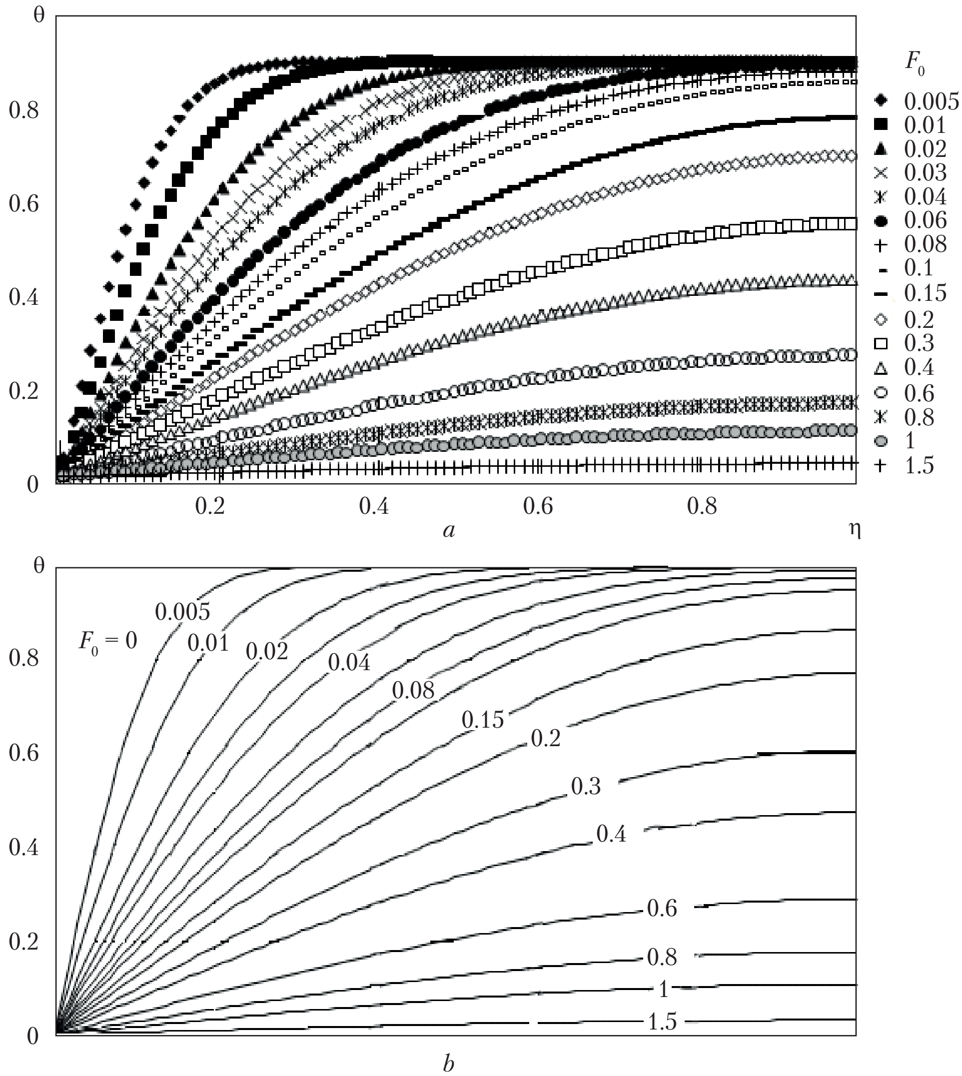

Fig. 2. Distribution of the temperature parameter in an infinite plate (problem 1): *a* — numerical calculation; *b* — analytical method

The analytical solution for the distribution of the temperature parameter is represented by an infinite series

$$\Theta = \sum_{n=1}^{\infty} A_n \sin[\mu_n \eta] / \exp(-\mu_n^2 F_0), \quad (21)$$

where the coefficients μ_n and A_n look like this:

$$\mu_n = n\pi, \quad (22)$$

$$A_n = (-1)^{n+1} \frac{2}{\mu_n}. \quad (23)$$

The results of comparison of analytical and numerical solutions are presented in Fig. 3.

Test problem 3. The process of heat exchange in an infinite plate with a constant distribution of initial temperature at a finite value of the heat transfer coefficient with the surrounding gaseous medium with temperature T_e is considered.

At the initial moment of time, the temperature in the plate has a constant value $T|_{\tau=0} = T_0$.

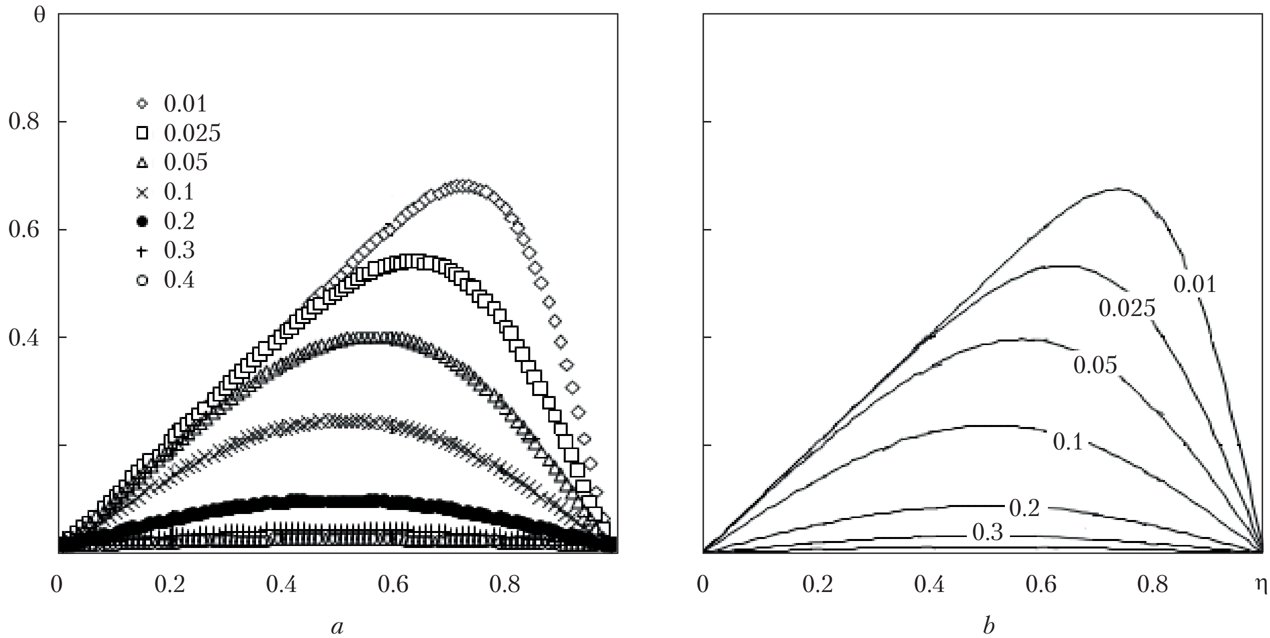

Fig. 3. Distribution of the temperature parameter in an infinite plate (problem 2): *a* — numerical calculation; *b* — analytical method

At one plate boundary the following condition is satisfied:

$$-\lambda \frac{\partial T}{\partial x}\bigg|_{x=0} = \alpha(T_e - T_{x=0}), \quad (24)$$

where ambient temperature T_e = const, λ is the thermal conductivity coefficient for the plate material, α is the heat transfer coefficient for the gas-solid system. On the other boundary the condition $\frac{\partial T}{\partial x}\Big|_{x=h} = 0$ is used. The analytical solution of the distribution of the temperature parameter is represented by an infinite series

$$\Theta = 1 - \sum_{n=1}^{\infty} A_n \cos[\mu_n(1-\eta)] / \exp(-\mu_n^2 F_0), \quad (25)$$

where the coefficients μ_n and A_n look like this:

$$\mathrm{ctg}\,\mu_n = \frac{1}{Bi}, \quad (26)$$

$$A_n = (-1)^{n+1} \frac{\left(2Bi\sqrt{\mu_n^2} + Bi^2\right)}{\left(\mu_n\left(\mu_n^2 + Bi^2 + Bi\right)\right)}. \quad (27)$$

The results of a comparison of analytical and numerical solutions under the condition that $\eta = 0$ and $\eta = 1$ are presented in Fig. 4 and Fig. 5.

The data from numerical calculations are in good agreement with analytical data, which allows the use of a mathematical model to solve the stated problem and reach the purpose.

Calculation of thermal conductivity in solids of complex shape. Based on a mathematical model, a computer subsystem for the engineering analysis of thermal conductivity in multiconnected solids with homogeneous thermophysical properties is created. Solids are subjected to cooling (heating) when instantly immersed in a heat-conducting gaseous medium. This subsystem is an integral part of the *Fire* research computer information system [4] that allows analyzing changes in the concentration of an explosive or toxic substance, overpressure and temperature in time and space in the computational area using personal computers in a practically acceptable time and predicting the consequences of exposure negative factors of accident releases to the environment.

Calculation in solid objects of simple shapes. Calculations of temperature fields are carried out in three-dimensional solids of primitive geometric shapes: sphere, cylinder, parallelepiped, prism

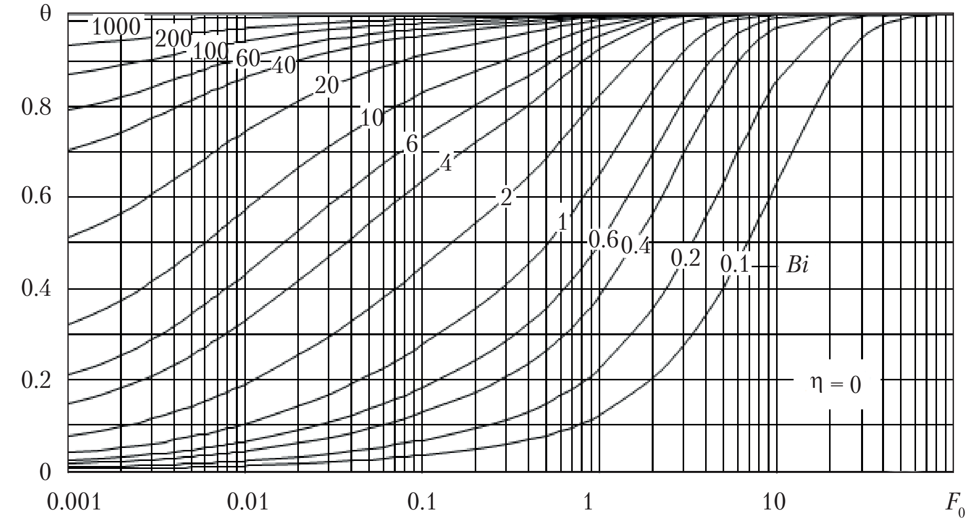

Fig. 4. Results of the analytical solution of the problem of heat transfer in an infinite plate (problem 3) at η = 0

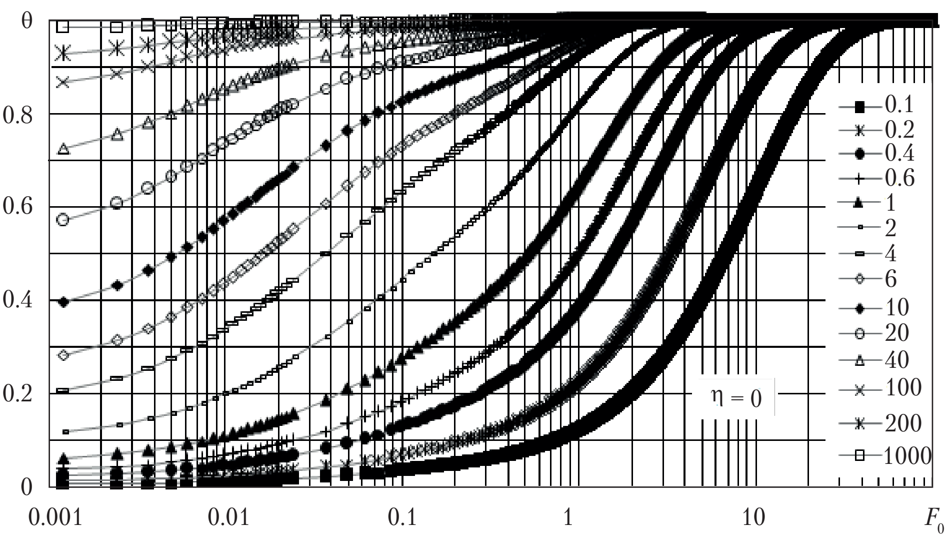

Fig. 5. Results of the numerical solution of the problem of heat transfer in an infinite plate (problem 3) at η = 0

with the base of a regular polyhedron and an arbitrary polygon. It is possible to arbitrarily arrange these figures in space relative to a given coordinate system.

To simplify the calculations, it is assumed that the surrounding gaseous medium is motionless and the intensity of heat transfer from the gas to the solid is infinitely large.

Calculation in objects with cavities. In addition to solid bodies, the developed computer system allows us to consider solid bodies with cavities filled with a gaseous medium. The previously listed geometric shapes are presented in a computer program as a system of related classes, which allows them to be used for constructing cavities in solids (Figs. 6, 7). The cooling results of a cylindrical body

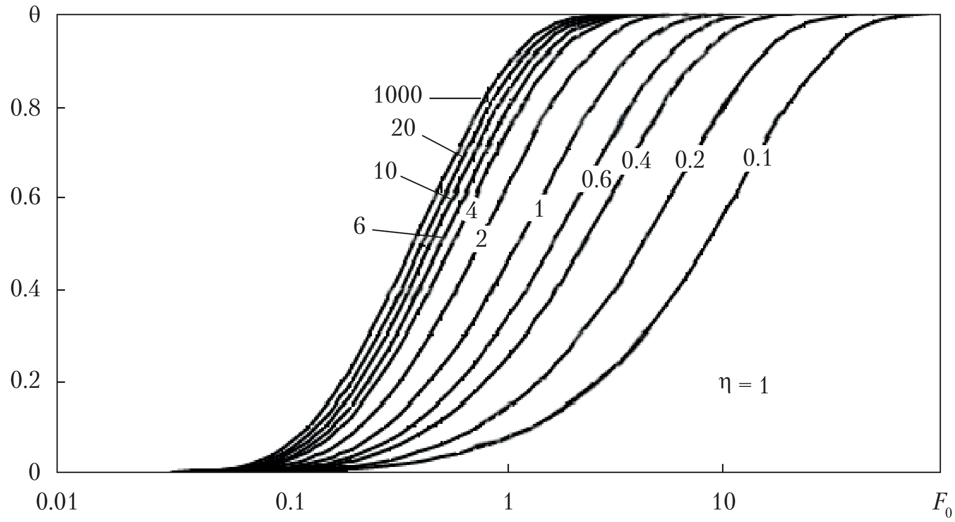

Fig. 6. Results of the analytical solution of the problem of heat transfer in an infinite plate (problem 3) at η = 1

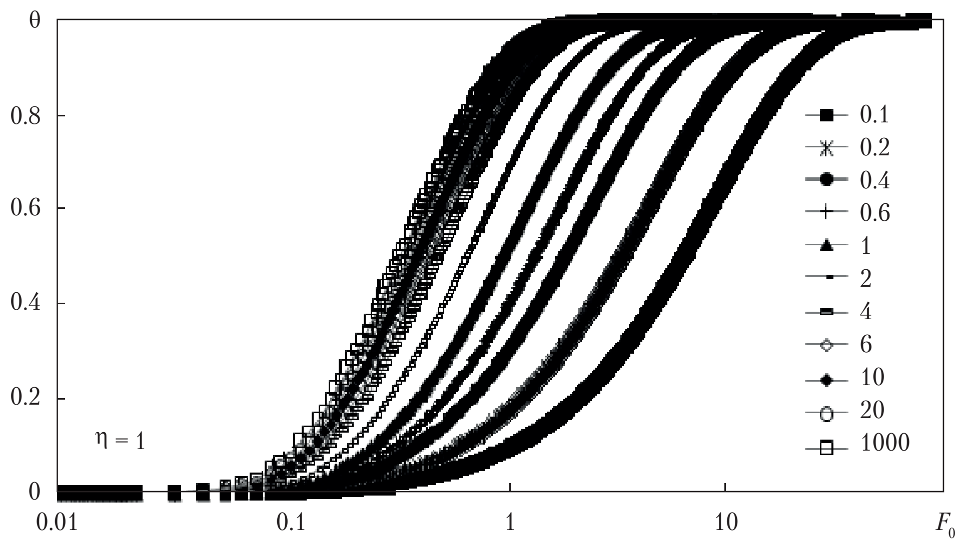

Fig. 7. Results of the numerical solution of the problem of heat transfer in an infinite plate (problem 3) at η = 1

with a parallelepiped-shaped cavity are presented in Fig. 8. It can be seen that the shape of solids and the presence of cavities of different geometric shapes significantly affect the nature of the temperature fields and the rate of the cooling process.

Calculation in objects of complex shapes. In actual engineering practice, solids subjected to thermal loading have complex shapes. Therefore, the computer system provides the ability to process solid bodies, the shape of which can be a set of bodies of the listed primitive shapes. The temperature field in the cross section of a body-combination of a prism with two parallelepipeds at a certain moment of the cooling process is presented in Fig. 9, *a*.

Often thermally stressed parts have a completely arbitrary shape, which cannot be a combination

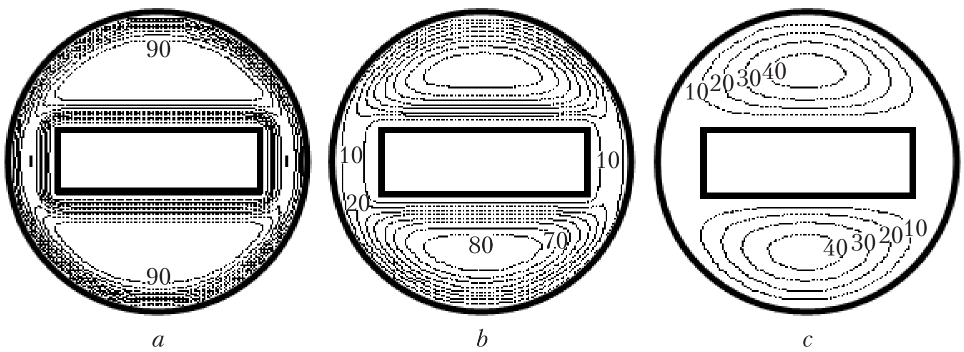

Fig. 8. Isotherms in the cross section of a cylinder with a cavity at different times of cooling: *a* — 0.5 s; *b* — 1.5 s; *c* — 2.5 s

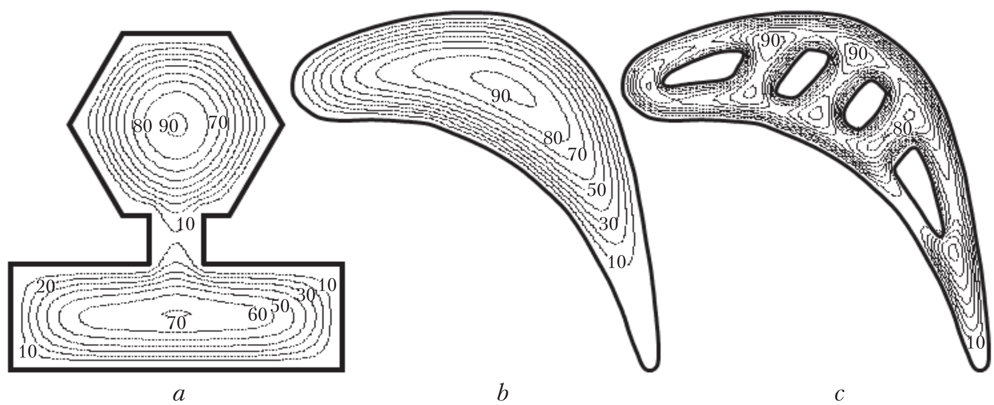

Fig. 9. Isotherms in the cross section of a body of complex shape at some point after the start of cooling: *a* — combination of bodies of simple shapes (1.49 s); *b* — solid turbine blade (8.5 s); *c* — turbine blade with cooling cavities (1.98 s)

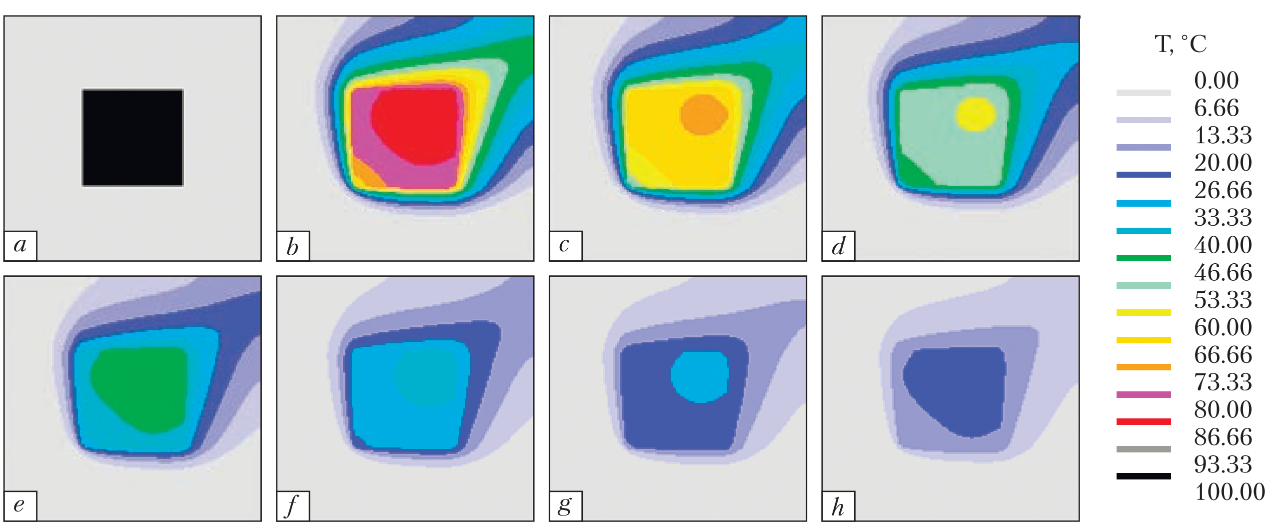

Fig. 10. Temperature fields in the cooling chamber at the following moments: *a* — 0 s; *b* — 10 s; *c* — 20 s; *d* — 30 s; *e* — 40 s; *f* — 50 s; *g* — 60 s; *h* — 70 s

of figures of simple geometric shapes. An example of such a body is a turbine blade. For this kind of bodies, the system suggests using bodies with an arbitrary polygon base. The coordinates of a flat section of a turbine blade form such a polygon. Model calculations of the cooling process of a typical turbine blade with a solid cross-section (Fig. 9, *b*) and with cooling cavities (Fig. 9, *c*) are carried out at infinitely high heat transfer intensity. It can be seen that the presence of cavities accelerates heat transfer.

Calculation of conjugate heat transfer. The adequacy of the developed mathematical model of conjugate heat transfer was carried out on the basis of a numerical solution of the test problem of cooling a hot (373 K) solid cubic steel body with a flow of heat-conducting gas (273 K) flowing at an angle of 45° at a speed of 10 m/s. To speed up the calculation, it was assumed that the level of heat transfer intensity, as well as the thermal conductivity of the gaseous medium and solid body, significantly exceed the physical real values.

The unsteady process of cooling a cubic solid body in the central section of a heat treatment chamber with cooling gas blowing is depicted in Fig. 10.

The results of numerical calculations have shown good agreement with the expected physical behavior, demonstrating acceptable accuracy. Notably, the resulting temperature fields exhibit a non-uniform distribution, which has been attributed to the presence of a colder, thermally conductive gaseous medium on the side of the oncoming flow — contrasting with the more uniform fields obtained for solids surrounded by a stationary, non-conductive gas. Incorporating the thermal conductivity of the gas has brought the simulation results closer to realistic physical conditions. This refinement has enhanced the model's applicability for evaluating the thermal efficiency of solid-body heat treatment chambers or assessing the stress state of structures subjected to combined thermal and pressure disturbances in the environment.

A three-dimensional mathematical model has been developed to simulate transient heat transfer processes in homogeneous, multiply connected solids of arbitrary geometry, surrounded by a thermally conductive gaseous medium. The model employs a finite-difference scheme to solve a three-dimensional system of gas dynamics equations, augmented by the internal energy conservation law for the solid. A unified, end-to-end computational algorithm has been formulated based on an explicit first-order finite-difference scheme, enabling the determination of thermophysical parameters for both the solid and the gas.

A dedicated computational system has been created to simulate unsteady heat transfer processes in solids of complex shapes. Validation of the model has confirmed its accuracy by comparison with established analytical solutions for several benchmark heat transfer problems. Numerical simulations have been carried out for the transient cooling of three-dimensional solid bodies with primitive geometric shapes, both with and without internal cavities filled with cooling gas. The temperature fields in a planar section of an uncooled and cooled turbine blade have been calculated and analyzed.

The obtained modeling results are applicable for subsequent evaluation of the stress distribution in solids exposed to thermal loading, particularly in regions with steep temperature gradients — for instance, near the epicenter of a gas explosion at high-risk industrial facilities.

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Ю.О. Скоб [1] (https://orcid.org/0000-0003-3224-1709),
М.Ю. Калініченко [1] (https://orcid.org/0000-0002-8685-065X),
І.О. Мамонтов [2] (https://orcid.org/0000-0002-7040-6247),
Р.І. Майборода [3] (https://orcid.org/0000-0002-3461-2959),
Н.В. Рашкевич [3] (https://orcid.org/0000-0001-5124-6068),
Ю.А. Отрош [3] (https://orcid.org/0000-0003-0698-2888)

[1] Національний аерокосмічний університет,
вул. Чкалова, 17, Харків, 61000, Україна,
+380 57 707 4080, khai@khai.edu
[2] Київський національний університет будівництва і архітектури,
проспект Повітряних Сил, 31, Київ, 03037, Україна,
+380 44 248 4901, Knuba_admin@ukr.net
[3] Національний університет цивільного захисту України,
вул. Чернишевська, 94, Харків, 61023, Україна,
+380 57 707 3403, nuczu@dsns.gov.ua

МАТЕМАТИЧНЕ МОДЕЛЮВАННЯ ТА ЧИСЕЛЬНИЙ АНАЛІЗ ТЕПЛООБМІНУ В ТВЕРДИХ ТІЛАХ СКЛАДНОЇ ФОРМИ

Вступ. Через надзвичайні ситуації можуть виникати вибухи, які супроводжуються виділенням температури та хвилями тиску, що руйнують конструкції на своєму шляху, спричиняючи пожежі.

Проблематика. Моделювання теплообміну в твердих тілах складної форми є актуальним завданням, оскільки прогнозування розподілу температурних полів можливо використовувати при проєктуванні захисних споруд. Тому створення нової математичної моделі, яка адекватно описує перехідні теплові процеси у твердих тілах, розробка ефективного методу розв'язання задачі та його реалізація у вигляді сучасної інформаційної системи, яка може бути використана в інженерних цілях для аналізу та прогнозування, є доцільним.

Мета. Математичне моделювання нестаціонарних температурних полів у твердих тілах в області значних температурних градієнтів, які виникають при аварійних вибухах газових сумішей.

Матеріали й методи. Чисельне моделювання нестаціонарних процесів теплообміну в багатозв'язаних твердих тілах складної форми, оточених теплопровідним газоподібним середовищем, виконано на основі єдиного кінцево-різницевого алгоритму.

Результати. Розглянуто спільну пряму задачу течії суцільного газоподібного середовища, теплообміну між газом і твердим тілом та теплопровідності всередині твердого тіла. Математична модель враховує просторовий характер перенесення маси, імпульсу й енергії, а також складну форму обтічних твердих тіл. Її перевірено через порівняння з аналітичними рішеннями тестових задач для нескінченної сталевої пластини. Отримано тривимірні температурні поля у просторових твердих тілах у вигляді різних примітивів, а також їхніх комбінацій. Проведено розрахунки теплообміну в лопатці турбіни суцільного перерізу, обладнаної порожнинами охолодження.

Висновки. Створену нову математичну модель може бути використано в інженерних цілях для аналізу та прогнозування. Тривимірні температурні поля можуть слугувати для оцінки термічного напруженого стану твердих тіл, а також характеристик міцності конструкцій, що знаходяться в зоні ударно-імпульсної дії високого надлишкового тиску внаслідок аварійного вибуху газових сумішей на промислових об'єктах.

Ключові слова: чисельне моделювання, теплообмін, теплопровідність, тверде тіло складної форми, ізотерми, температурне поле.