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THREE-DIMENSIONAL COMPUTER MODELING OF COOLING OF A CASTING AND SELECTION OF THE RUNNER OF A GATING SYSTEM BASED ON THE HEAT CONDUCTION EQUATION

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Consideration is given to a mathematical model for computer modeling of thermal processes of cooling of alloys in gating systems that uses a cellular-automaton representation. The results of optimization of the runner dimensions for different castings obtained based on a software package that realizes three-dimensional computer modeling of thermal processes are given.

As a rule, the design and optimization of gating systems by analytical methods are impossible because of the complex shape of the castings and the spatial distribution of thermal processes in the system.

One of the simplest and universal mathematical models for a numerical calculation of similar systems is a cellular automaton. Because of the rapid growth of the productivity of computer technology these models may become widespread in investigating processes in continua [1] (thermal processes, fluid and gas flows, etc. [2]). The idea of cellular automata was formulated independently by J. von Neuman and K. Zusse in the late 40s. J. von Neuman used them subsequently to provide more realistic models of the behavior of complex spatially extended systems [3].

It is customary to use the name of "cellular automata" to refer to networks of elements that change their states at discrete instants by a certain law, depending on the state of the element itself and that of its closest neighbors at the previous instant. In homogeneous cellular automata the elements of the network, the links between them, and the rules of transition to a new state are the same.

To consider physical continua, they should be limited to regular networks whose elements occupy the nods of a regular cubic grid. In our case, the elements were segments of cubic shape and of the same size, into which the entire space of the modeled system was broken. The state of the element is the temperature in this segment, the material that fills this segment (a melt or a mold), and the quantity of heat released in the volume of this segment in metal crystallization.

The representation of a real physical system by a cellular-automaton model corresponds, from the mathematical point of view, to a transition from the description of a system in differential equations to a finite-difference scheme. In our case, in calculation of temperature-time dependences use was made of a three-dimensional differential heat-conduction equation [5]

$$\frac{\partial T}{\partial \tau} = \frac{\lambda}{c\rho}\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2}\right) + \frac{F}{c\rho}. \tag{1}$$

With allowance for the thermal conductivity and the heat capacity of the material as functions of temperature Eq. (1) has the form

$$\frac{\partial T}{\partial \tau} = \frac{1}{c(T)\rho}\left(\frac{\partial\left(\lambda(T)\frac{\partial T}{\partial x}\right)}{\partial x} + \frac{\partial\left(\lambda(T)\frac{\partial T}{\partial y}\right)}{\partial y} + \frac{\partial\left(\lambda(T)\frac{\partial T}{\partial z}\right)}{\partial z}\right) = \frac{F}{c(T)\rho}. \tag{2}$$

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The quantity $T(\tau)$ from Eq. (2) was determined based on the finite-difference scheme [6], under which the volume was broken into elements of cubic shape with length $\Delta x = 10$ mm, width $\Delta z = 10$ mm, and height $\Delta y = 10$ mm. The increment in temperature in one element after the time interval $\Delta\tau = 0.5$ sec was determined by the formula

$$\Delta T(x, y, z) = \frac{\Delta\tau}{c(T(x, y, z))\rho} \times$$

$$\times \left(\frac{\lambda_{x+\Delta x,y,z} \frac{T(x, y, z) - T(x + \Delta x, y, z)}{\Delta x} - \lambda_{x-\Delta x,y,z} \frac{T(x, y, z) - T(x - \Delta x, y, z)}{\Delta x}}{\Delta x} + \right.$$

$$+ \frac{\lambda_{x,y+\Delta y,z} \frac{T(x, y + \Delta y, z) - T(x, y, z)}{\Delta y} - \lambda_{x,y-\Delta y,z} \frac{T(x, y, z) - T(x, y - \Delta y, z)}{\Delta y}}{\Delta y} +$$

$$+ \frac{\lambda_{x,y,z+\Delta z} \frac{T(x, y, z + \Delta z) - T(x, y, z)}{\Delta z} - \lambda_{x,y,z-\Delta z} \frac{T(x, y, z) - T(x, y, z - \Delta z)}{\Delta z}}{\Delta z} +$$

$$\left. + F(x, y, z)\,\Delta x\Delta y\Delta z \right) . \tag{3}$$

The thermal conductivities between two neighboring elements were determined as

$$\lambda_{x+\Delta x,y,z} = \frac{\lambda(T(x, y, z))\,\lambda(T(x + \Delta x, y, z))}{\lambda(T(x, y, z)) + \lambda(T(x + \Delta x, y, z))} ; \tag{4}$$

similarly, they were determined between the remaining couples of elements.

The bulk density of the power of heat release in crystallization was calculated by the ratio

$$F(x, y, z) = \begin{cases} \left(1 - \frac{Q(x, y, z)}{Q_{cr}}\right) \xi , & \text{if } T(x, y, z) \le T_{cr} \text{ and } Q(x, y, z) < Q_{cr} , \\ 0 , & \text{if } T(x, y, z) > T_{cr} \text{ or } Q(x, y, z) \ge Q_{cr} , \end{cases} \tag{5}$$

where $Q(x, y, z)$ is the quantity of heat released in the element with the coordinates (x, y, z) up to the current moment and changes with every time step by the formula

$$Q(x, y, z, \tau + \Delta\tau) = Q(x, y, z, \tau) + F(x, y, z)\,\Delta x\Delta y\Delta z\Delta\tau . \tag{6}$$

Thus, the numerical solution of the system of differential equations simulationally models a cellular-automaton [7]. The adoption of principles of simulation modeling makes it possible, apart from the evaluation of the effect of the parameters of the system, to observe the behavior of the system's components for a certain period of time and to control the course of the process by slowing down or accelerating the phenomena in the course of simulation, and by changing some parameters.

The developed program simulator of cellular-automata allows the creation of a three-dimensional data array of arbitrary dimensions depending on the number of elements, into which the modeled space is broken (each element of the space corresponds to an element of the array with the same coordinates). The user is also offered to assign the number and size of the variables describing the state of one element. To operate with such a big array of structured data the program simulator of cellular-automata identify the value of the element's parameter with some color and puts the graphical image of any or several cross sections of the modeled space onto the display. The bigger the numerical value of a parameter, the closer the cell's color to red; the smaller it is, the closer it is to blue. A black-and-white version is possible: the bigger the numerical value of a parameter, the closer the cell's

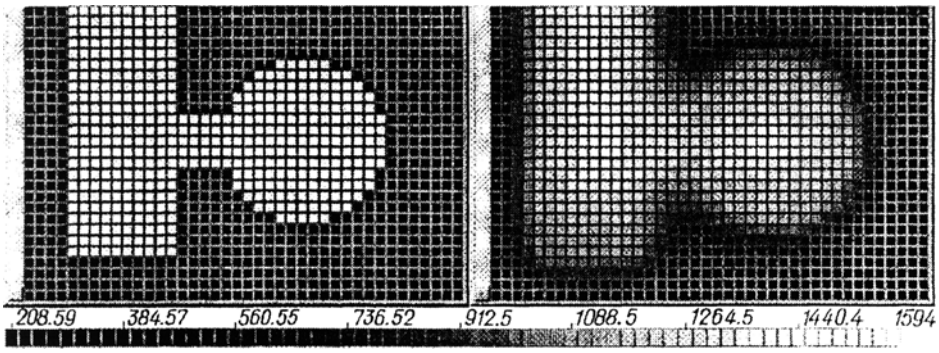

Fig. 1. Computer image of the cross sections of a temperature field of a gating system for a spherical casting at the beginning of the process of cooling of metal (on the left), after 830 sec of the model time (on the right), and the scales of the agreement between the color of a cell and the temperature in °C (at the bottom).

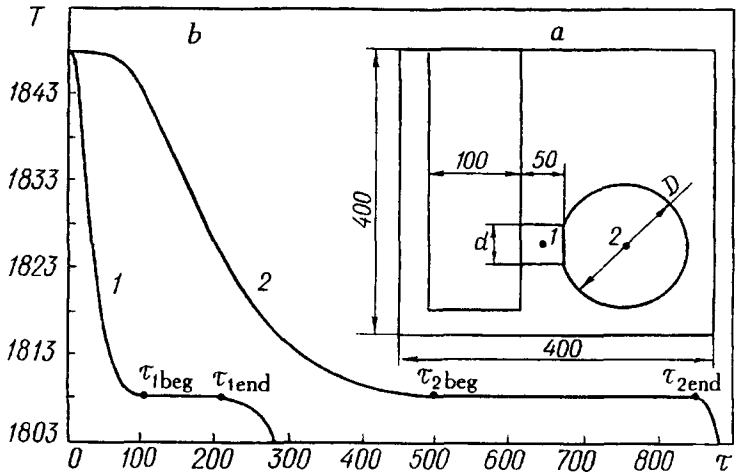

Fig. 2. Scheme of a model gating system for production of a casting in the shape of a sphere (a) (the size of regions in millimeters) and temperature-time dependences of points 1 and 2 (b) computed based on solution of a three-dimensional heat-conduction equation. T, K; τ, sec.

color to white; the smaller it is, the closer it is to black. For example, Fig. 1 represents images of cross sections of the temperature field of a gating system at the beginning of the process of metal cooling (on the left) and 830 sec later (on the right). The representation of a big volume of information (several thousand elements in a cross section) in the form of visual images (color fields) allows the researcher not only to perceive more information per unit time, but also to do it at a higher qualitative level, i.e., to directly observe the processes modeled. The assignment of initial states of elements or their change in the process of modeling resembles drawing objects with the help of a graphical editor. This accessibility of data and the possibility of perceiving simultaneously a great body of information simplify qualitatively a computational experiment and the processing of its results. In case modeling requires significant time there is a possibility of recording frames of images of cross sections in the process of modeling with the aim of their repeated accelerated viewing.The package contains a program to construct curves of variation in the parameters of the required elements with time. The essence of the process of modeling by this program is a successive selection of the array's elements and their change as a function of their current state and the state of the neighbors. The law of change is formed separately from the main program in the form of a library of a dynamic arrangement using any high-level programming language compiler.

As an example of the use of the above methods and programs we consider the problem of selecting the diameter of the runner d to obtain a sphere-shaped casting.

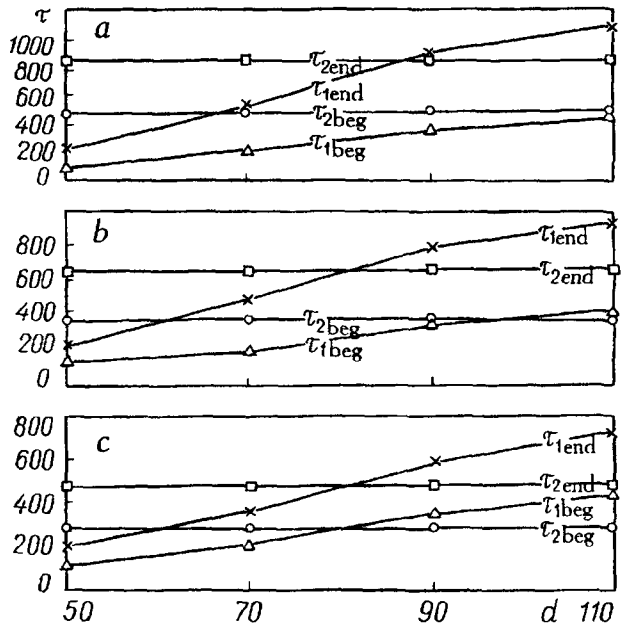

Fig. 3. Nomograms for determination of the optimum dimensions of a runner (d) for different dimensions of spherical castings [a) D = 150 mm, b) 130, c) 110]. d, mm.

Figure 2a presents the scheme of a simple gating system for obtaining a sphere-shaped casting of diameter D. When calculations were made the following parameters of the material of the mold were used: the heat capacity of the mold was 2.09 J/(m^3·K); its thermal conductivity was 4.4 Wt/(m·K). The calculations were made for an iron melt (thermophysical properties are taken from [8]).

The modeling resulted in obtaining this gating system's temperature field, which varies with time (Fig. 1 for d = 50 mm and D = 150 mm). In the process of crystallization of the metal, its volume decreases and the casting develops "hollows" and "gas cavities." To prevent this from happening the melt should pass through the runner as the crystallization proceeds. If the runner's channel becomes crystallized earlier than the casting does, it won't be able to compensate for the shortage of metal in the casting. This is illustrated by the temperature-time dependences for points 1 and 2 (the middle section and the center of a sphere in Fig. 2a) shown in Fig. 2b.

Similar computational experiments were conducted for sphere diameters D of 110, 130, and 150 mm with runner diameters d of 50, 70, 90, and 110 mm. Figure 3 shows the dependences of the time of the beginning and the end of crystallization of the runner and the casting for different D and d. The given results show that for the sphere with a diameter of 150 mm the runner must have a diameter of over 89 mm (Fig. 3a), for the sphere with a diameter of 130 mm – over 81 mm (Fig. 3b) and for the sphere with a diameter of 110 mm – also over 81 mm (Fig. 3b).

The low cost of a computational experiment (it is enough to just have a personal computer), the short time required for data preparation (it is required to use the "mouse" to "draw" the necessary shape on the computer's screen), and the simplicity of representation (in the form of a graphical image) and of the analysis of the results make it possible to expect wide use of the above methods and programs in the machine-building industry.

NOTATION

T, temperature; λ, thermal conductivity of material; c, specific heat of material; ρ, density of material; x, y, and z, Cartesian coordinates; $T(x, y, z)$, temperature of the isolated element with the coordinates (x, y, z); Δx, Δy, and Δz, dimensions of the element of the modeled space; τ and $\Delta\tau$, time and the time step of modeling; $T(\tau)$, temperature-time dependence of the individual element; $c(T)$ and $\lambda(T)$, specific heat and thermal conductivity at temperature T; $\lambda_{x+\Delta x,y,z}$, $\lambda_{x-\Delta x,y,z}$, $\lambda_{x,y+\Delta y,z}$, $\lambda_{x,y-\Delta y,z}$, $\lambda_{x,y,z+\Delta z}$, and $\lambda_{x,y,z-\Delta z}$, thermal conductivities between

the elements with the coordinates (x, y, z) and $(x + \Delta x, y, z)$, (x, y, z) and $(x - \Delta x, y, z)$, etc.; $F(x, y, z)$, bulk density of the power of heat release in crystallization; Q_{cr}, maximum quantity of heat released in crystallization of metal in the volume $\Delta x \Delta y \Delta z$ (for 1 cm^3 of iron, $Q_{cr} = 1967.6$ J); T_{cr}, crystallization temperature (for iron, $T_{cr} = 1535$ K); ξ, empirical coefficient determined for this metal; τ_{1beg} and τ_{1end}, time of the beginning and the end of crystallization of the runner; τ_{2beg} and τ_{2end}, the same for the casting.

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