

A METHOD OF NUMERICAL SOLUTION OF ONE-DIMENSIONAL STEFAN PROBLEMS OF TWO TYPES

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A one-dimensional conjugate problem of heat transfer with phase transitions of two types (with interfaces of two phases and with a two-phase zone) is solved by a finite difference method based on the general initial heat conduction equation written with the Dirac delta function. A calculating scheme is developed using a nonuniform spatial net with floating nodes and the method of oppositely directed pivots.

The consideration of contingent emergencies of nuclear reactors with melting of the active zone necessitates mathematical modeling of the heat transfer with phase transitions in the reactor materials. As a rule, one has to solve a multifront problem, viz., a conjugate problem of heat transfer with the presence of several fixed and moving boundaries.

A change in the state of aggregation is accompanied, strictly speaking, by the presence of a buffer zone between two adjacent phases with a temperature drop equal to the drop between the liquids and solidus lines. Such a two-phase zone, consisting partly of a liquid phase and partly of a solid phase, occupies a significant volume fraction of the medium under certain conditions (for example, with radiative transfer within the substance volume [1] or in solidification of a binary melt [2]). A vast two-phase zone also arises when there is an internal heat release distributed over the medium volume, for example, in the fuel core of a heat-releasing element (fuel element) of a nuclear reactor. A two-phase layer narrows in the limiting case, and then the problem may be reduced to a classical one that assumes the presence of a phase front between zones with different states of aggregation.

A good deal of attention is given in the literature to the methods of solving the Stefan problem in a classical statement. For individual simple cases, there are exact analytic solutions, for example, that reported in [3, 4], and also approximate analytic solutions, for example, those presented in [3]. The greatest development was extended to numerical methods of solving the Stefan problems, chiefly as applied to problems of permafrost science, geology, and metallurgy. Some methods of numerical solution are described in [5]. Most familiar numerical methods are suitable for simple problems characterized by the presence of a single interface of two phases, including the solution described in [6]. Work [7] proposed a method of numerical solution of multifront one-dimensional Stefan problems. There are also publications concerning the solution of a nontraditional Stefan problem [1, 2]. One of the methods of solution with a strongly discontinuous dependence of the specific-heat function in the vicinity of the two-phase zone, satisfying the energy balance condition, is used in [8]. There are numerical solutions of multidimensional problems, for example, of a problem with a flat oblique front [4]. Numerical methods for solving problems of heat transfer with phase transitions are described in [9].

The presence of moving boundaries requires the use of appropriate calculating schemes. The order of accuracy of a scheme with a uniform spatial net and a fixed temporal step decreases with the appearance of a moving discontinuity [4]. For improvement of the calculation accuracy the spatial net must be more close-meshed in this case. A calculating scheme with a variable temporal step and a boundary displacement by one spatial node of a uniform net is more workable for Stefan problems [5, 10]. For a multifront problem, however, this scheme loses its advantage to some extent. In this sense a calculating scheme using fractional spatial steps for the displacement of the phase front at each temporal step (which is fixed) must be more suitable [5]. Here, the coordinate of the moving boundary does not coincide with the location of any node of the spatial net. Some numerical solutions, for

example, those reported in [6, 7], employ calculating nets containing, apart from fixed nodes, moving (floating) ones, whose coordinates correspond to the locations of phase fronts. Such a method admits any number of moving boundaries without a decrease in the approximation accuracy.

The current study suggests a numerical method for a one-dimensional conjugate (multizonal) problem of heat transfer with phase transitions of two types (with interfaces of two phases and with a two-phase zone). The problem is solved in a formulation generalized for Cartesian, cylindrical, and spherical coordinate systems. The number of calculation regions is arbitrary, with any types of boundary conditions (BC), and several calculating models are used for each of four BC kinds (among them are those specific for the range of problems considered). In each of the regions, the movement of both the interfaces of two phases and the boundaries of a two-phase zone (of one or simultaneously two boundaries) may be examined. The number of interfaces, including those within one calculated region, is not limited (the problem is multifront). Such a moving front can also be situated on the boundary of the calculation region, for example, in melting or solidification at the interface of a solid and a moving liquid mass. The initial equation is solved numerically using a finite difference method with the application of a nonuniform spatial net with floating nodes, as in the solution of [6]. In the solution put forward in the present work a discrete analog, describing heat transfer inside single-phase zones or a two-phase zone and the movement of clearly separable fronts (of the interfaces of two phases or the boundaries of a two-phase zone), is obtained from one initial equation written, similarly to [4], with the Dirac delta function. Furthermore, in the present solution the method of oppositely directed pivots [11] is used.

The heat transfer within single-phase zones is described in a one-dimensional formulation, common to the three coordinate systems, by the following heat conduction equation:

$$c(r, T) \frac{\partial T(r, t)}{\partial t} = \frac{1}{r^k} \frac{\partial}{\partial r} \lambda(r, T) r^k \frac{\partial T(r, t)}{\partial r} + q_v(r, t), \quad (1)$$

where $k = 0$ in a Cartesian coordinate system, $k = 1$ in a cylindrical, and $k = 2$ in a spherical.

The temperature at the interface is equal to the temperature of the phase transition, and the heat fluxes are discontinuous. The conditions at such a classical interface (the Stefan conditions) in a one-dimensional case have the form

$$\begin{aligned} -\lambda(r, T) \frac{\partial T(r, t)}{\partial r} \Big|_{r=y-} + \lambda(r, T) \frac{\partial T(r, t)}{\partial r} \Big|_{r=y+} = \\ = \pm R_m \frac{\partial y(t)}{\partial t}; \quad T(y, t) = T_m. \end{aligned} \quad (2)$$

Having introduced the Dirac delta function with the aim of defining the heat transfer inside a continuous medium and the movement of several moving interfaces by one common equation we write the heat conduction equation (1) as

$$\begin{aligned} \left[c(r, T) \pm \sum_{p=1}^n R_m^p \delta(T - T_m^p) \right] \frac{\partial T(r, t)}{\partial t} = \\ = \frac{1}{r^k} \frac{\partial}{\partial r} \lambda(r, T) r^k \frac{\partial T(r, t)}{\partial r} + q_v(r, t). \end{aligned} \quad (3)$$

On the left side of Eq. (3) a plus sign is written for $\partial T(r, t)/\partial r < 0$ and a minus sign in the opposite case. Clearly, when the coordinate r does not coincide with the coordinate of any interface (y_p), we have all zero terms of the latter equation that incorporate the delta function; here Eq. (3) reduces to Eq. (1). At the p -th moving interface with a temperature T_m^p , we obtain the corresponding nonzero term (the remaining ones, if there are several such fronts, are zero at this point); as a result, the equation will express the law of motion of the p -th interface.

The heat transfer in the case with a two-phase zone is, as a rule, described approximately by a heat conduction equation of type (1) but with a strongly discontinuous dependence of the specific heat at its boundaries.

Here, the value of the specific heat inside the zone includes the latent heat of a phase transition such as, for example, that in [12]:

$$c_{SL} = R_m/\Delta T + [c_S(T_m) + c_L(T_m + \Delta T)]/2. \quad (4)$$

The heat fluxes on moving boundaries of the two-phase zone are constant.

As the initial equation for obtaining a discrete analog, common to the two types of phase transitions considered, the current work uses Eq. (3), in which the terms containing a delta function with the coefficients R_m relate to classical interfaces, whereas, for a two-phase zone, the latent heat of the phase transition is accounted for in the specific heat defined by Eq. (4). A numerical solution is obtained without preliminary smoothing of the delta function in a certain temperature range, as was done in the approximate solution [4] for the classical Stefan problem.

A conservative finite difference scheme (discrete analog) for a problem of heat conduction with discontinuous coefficients can be obtained by an integro-interpolation method (balance method) [4]. A purely implicit scheme that is absolutely stable [11, 13] is used. A discrete analog of the generalized equation (3) that is obtained for a nonuniform spatial net using piecewise-constant temperature profiles on control segments is of the form

$$\begin{aligned} c_i^{j+1} (T_i^{j+1} - T_i^j) \pm R_m^i \frac{(y_p^{j+1})^{k+1} - (y_p^j)^{k+1}}{(k+1)\varphi_i(k)\tilde{h}_i} = \\ = - \frac{\tau}{\tilde{h}_i \tilde{h}_{i+1}} \frac{r_{i+1/2}^k}{\varphi_i(k)} \lambda_{i+1/2}^{j+1} (T_i^{j+1} - T_{i+1}^{j+1}) + \\ + \frac{\tau}{\tilde{h}_i \tilde{h}_i} \frac{r_{i-1/2}^k}{\varphi_i(k)} \lambda_{i-1/2}^{j+1} (T_{i-1}^{j+1} - T_i^{j+1}) + \tau q_v^{i,j+1}, \end{aligned} \quad (5)$$

where

$$\begin{aligned} \tau &= t_{j+1} - t_j; \quad T_i^{j+1} = T(r_i, t_{j+1}); \quad y_p^j = y_p(t_j); \\ \tilde{h}_i &= r_i - r_{i-1}; \quad \tilde{h}_i = (h_i + h_{i+1})/2; \quad r_{i-1/2} = r_i - h_i/2; \\ \lambda_{i-1/2}^{j+1} &= [\lambda(r_{i-1}, T_{i-1}^{j+1}) + \lambda(r_i, T_i^{j+1})]/2; \\ c_i^{j+1} &= c(r_i, T_i^{j+1}); \quad q_v^{i,j+1} = q_v(r_i, t_{j+1}); \\ \varphi_i(k) &= 1 \quad \text{at } k=0; \quad \varphi_i(k) = r_i + (h_{i+1} - h_i)/4 \quad \text{at } k=1; \\ \varphi_i(k) &= r_i^2 + r_i(h_{i+1} - h_i)/2 + (h_{i+1}^2 - h_i h_{i+1} + h_i^2)/12 \quad \text{at } k=2. \end{aligned}$$

In this equation, $R_m^i = R_m^p$ and $r_i(t_{j+1}) \equiv y_p^{j+1}$, if $y_p^j = r_i(t_j)$ (for $p = 1, \dots, n$). With no interface inside the considered i -th control segment ($y_p \neq r_i$), $R_m^i = 0$ in Eq. (5), i.e., the term with the coefficient R_m is absent. When the interface or one of the boundaries of the two-phase zone is determined in the i -th control segment, the nonstationary term will tend to zero, if its coordinate is chosen correctly.

For control segments with moving boundaries, the specific heat is defined as

$$c_i^{j+1} = \frac{c_{i-}^{j+1} \varphi_{i-}(k) \tilde{h}_i/2 + c_{i+}^{j+1} \varphi_{i+}(k) \tilde{h}_{i+1}/2}{\varphi_i(k)}, \quad (6)$$

where $c_{i-}^{j+1} = c(r_{i-}, T_i^{j+1})$, $c_{i+}^{j+1} = c(r_{i+}, T_i^{j+1})$, and the coefficients $\varphi_{i-}(k)$ and $\varphi_{i+}(k)$ are determined from the corresponding equations.

Alternatively, the discrete analog (5) of the heat conduction equation is written in the form [4]

$$A_i T_{i-1}^{j+1} - C_i T_i^{j+1} + B_i T_{i+1}^{j+1} + F_i = 0, \quad (7)$$

the coefficients of which are defined as

$$\begin{aligned}
A_i &= \frac{\tau}{\tilde{h}_i \tilde{h}_i} \lambda_{i-1/2}^{j+1} \frac{(r_i - h_i/2)^k}{\varphi_i(k)}; \quad B_i = \frac{\tau}{\tilde{h}_i \tilde{h}_{i+1}} \lambda_{i+1/2}^{j+1} \frac{(r_i + h_{i+1}/2)^k}{\varphi_i(k)}; \\
C_i &= A_i + B_i + c_i^{j+1}; \quad F_i = c_i^{j+1} T_i^j + \\
&+ \tau q_v^{i,j+1} \mp R_m^i \frac{(y_p^{j+1})^{k+1} - (y_p^j)^{k+1}}{(k+1) \varphi_i(k) \tilde{h}_i}.
\end{aligned} \tag{8}$$

This discrete analog is valid for all nodes of the spatial net, both fixed and moving (a uniform scheme). Its distinctive feature is primarily that, in the expression for one of its coefficients (F_i) there arises an additional term accounting for the energy consumption/liberation on the phase transition localized at the i -th node.

The boundary conditions of the calculation regions are written in discrete form as [11]

$$T_{N_1}^{j+1} = \kappa_1 T_{N_1+1}^{j+1} + \nu_1; \quad T_{N_2}^{j+1} = \kappa_2 T_{N_2-1}^{j+1} + \nu_2, \tag{9}$$

where the coefficients κ_1, ν_1 , and κ_2, ν_2 , are determined from equations appropriate to the kind of BC.

A combination of the pivot and iteration methods [11] is employed to solve the nonlinear system of algebraic equations (7) and (9). The methods of right and left pivots are used [11], in which the temperatures of neighboring nodes are related by the recursive equations

$$T_i^{j+1} = \alpha_{i+1} T_{i+1}^{j+1} + \beta_{i+1}; \quad T_{i+1}^{j+1} = \alpha_{i+1} T_i^{j+1} + \beta_{i+1}, \tag{10}$$

where the pivot coefficients α_i and β_i are determined from the corresponding equations. In the present numerical solution for the problem of phase transitions of both types, the method of oppositely directed pivots [11] is used, for which the right and left pivots are performed relative to the moving interfaces. The expression for the temperature on moving boundaries is obtained from discrete analog (7) and pivot equations (10) and has the form

$$T_i^{j+1} = \frac{F_i + A_i \beta_i + B_i \beta_{i+1}}{C_i - A_i \alpha_i - B_i \alpha_{i+1}}. \tag{11}$$

The coordinates of phase fronts are found using an iteration method. Here, the coordinate of the moving boundary is redetermined (inside a cycle of the above-mentioned iterations) several times until the required difference of the temperature, found using Eq. (11), from that specified for this boundary is attained. When the second moving boundary appears in the calculation region, such iterations are repeated alternately for both fronts, whereupon the temperatures (starting from the second front) at the remaining nodes of the spatial net, including those on the first moving boundary, are calculated using Eq. (10). Because both expression (11) and the coefficients of the pivot equation are obtained in the present solution from the common initial equation (7) that takes into account the latent heat of phase transitions at the interfacial nodes of the spatial net, the interfacial temperatures calculated from these expressions will not differ, which ensures convergence of the iteration process.

The presented algorithm of numerical solution for the conjugate problem of heat conduction with phase transitions of two types is realized in the TRAMS computation program in the FORTRAN language for the ES computer.

For testing the accuracy of the numerical method, the results computed by the TRAMS program are compared with the predictions from the exact analytic solution. The solution for the classical self-similar problem of freezing of moist ground (a semi-infinite medium with the surface BC of the 1st kind), reported in [3], defines the law of motion of the liquid-solid interface as $y = \gamma\sqrt{t}$, where γ is a constant, whose value is determined by the relation

$$\frac{\lambda_L (T_c - T_m) \exp\left(-\frac{\gamma^2}{4a_L}\right)}{\sqrt{a_L} \Phi\left(\frac{\gamma}{2\sqrt{a_L}}\right)} +$$

TABLE 1. Coordinates of the Solid-Liquid Interfaces in a Steel Plate for a Self-Similar Problem

t, sec	1	2	3	4	5
y, cm ($T_0 = 1540^\circ\text{C}$)	0.25760	0.36430	0.44617	0.51520	0.57601
	0.25430	0.36303	0.51681	0.51660	0.57824
y, cm ($T_0 = 350^\circ\text{C}$)	0.10131	0.14320	0.17548	0.20262	0.22654
	0.10370	0.14597	0.17788	0.20545	0.22938

Note: The upper value pertains to the exact solution, and the lower value, to the numerical.

TABLE 2. Temperatures at the Boundaries of a Cylindrical Element at the Instant the Movement of the Second Front Terminates

$\Delta T, ^\circ\text{C}$	40	50	100	200	300
$T_{N1}, ^\circ\text{C}$	2981.5	2988.8	3023.5	3100.6	3184.8
	2993.6	3000.7	3033.4	3107.2	3189.1
$T_{N2}, ^\circ\text{C}$	2890.4	2900.6	2950.3	3050.2	3150.4
	2883.5	2895.1	2945.3	3047.1	3148.6

Note: The upper value pertains to the calculation with two moving fronts, and the lower value, to the control calculation.

$$+ \frac{\lambda_s (T_0 - T_m) \exp\left(-\frac{\gamma^2}{4a_s}\right)}{\sqrt{a_s} \left\{1 - \Phi\left(\frac{\gamma}{2\sqrt{a_s}}\right)\right\}} = -R_m \gamma \frac{\sqrt{\pi}}{2}, \quad (12)$$

where Φ is the error integral.

For test calculations, we selected a problem of melting of a semi-infinite medium at a constant higher temperature on the finite boundary that has the same analytic solution. In this case, the constant γ is determined by a relation differing from Eq. (12) only by the sign of the right side.

Table 1 gives results calculated from the exact and numerical solutions for two cases: 1) the initial temperature of the melted material (a steel plate) is equal to the melting temperature ($T_0 = T_m$) and 2) the initial temperature of the plate is below the melting temperature ($T_0 = 350^\circ\text{C}$). In the first case, the temperature in the solid zone does not change and the law of motion of a phase front in a semi-infinite medium is valid (up to plate melting) also for a medium of any finite dimension. In the second case, there is no effect of the finite dimension of a solid layer until the temperature on the outer boundary starts rising. The following thermophysical properties of steel are assumed: $\lambda_L = 10 \text{ W}/(\text{m} \cdot \text{deg})$; $\lambda_s = 30 \text{ W}/(\text{m} \cdot \text{deg})$; $a_L = 1.85 \cdot 10^{-6} \text{ m}^2/\text{sec}$; $a_s = 5.56 \cdot 10^{-6} \text{ m}^2/\text{sec}$; $T_m = 1540^\circ\text{C}$; and $R_m = 21 \cdot 10^8 \text{ J}/(\text{m}^3 \cdot \text{sec})$. The boundary temperature is $T_c = 2850^\circ\text{C}$. With such parameters, the following constants of the exact solution are obtained: 1) $\gamma = 0.2576$ and 2) $\gamma = 0.10131$. The initial step of the spatial net in the numerical solution is $h = 0.05 \text{ cm}$, the temporal step is $\tau = 0.1 \text{ sec}$, and the accuracy of the temperature calculation at the net nodes is 10^{-6} . It is evident from the table that the results of numerical and analytic solutions coincide with a precision of two significant figures. The coordinate of the solid-liquid interface at each temporal step is found in a smaller number of iterations than with the method, in which the law of motion of the interface is expressed by a discrete analog of Stefan's condition [6]. Convergence of the iteration process is improved due to the influence of the nonstationary term of the heat conduction equation, from which expression (7) with coefficients (8) is derived.

To check the accuracy of the numerical method on a problem with two concurrently moving boundaries of a two-phase zone, we calculated the temperature fields in a cylindrical element (the core of a fuel element 5.9 mm in diameter [14] with an inner axial opening 2 mm in diameter) under an adiabatic condition on the surface. In the calculations we adopted: $q_v = 2.06 \cdot 10^6 \text{ kW}/\text{m}^3$, $\lambda_s = 2.9 \text{ W}/(\text{m} \cdot \text{deg})$; $c_s = 6.43 \cdot 10^6 \text{ J}/(\text{m}^3 \cdot \text{deg})$; and $T_m =$

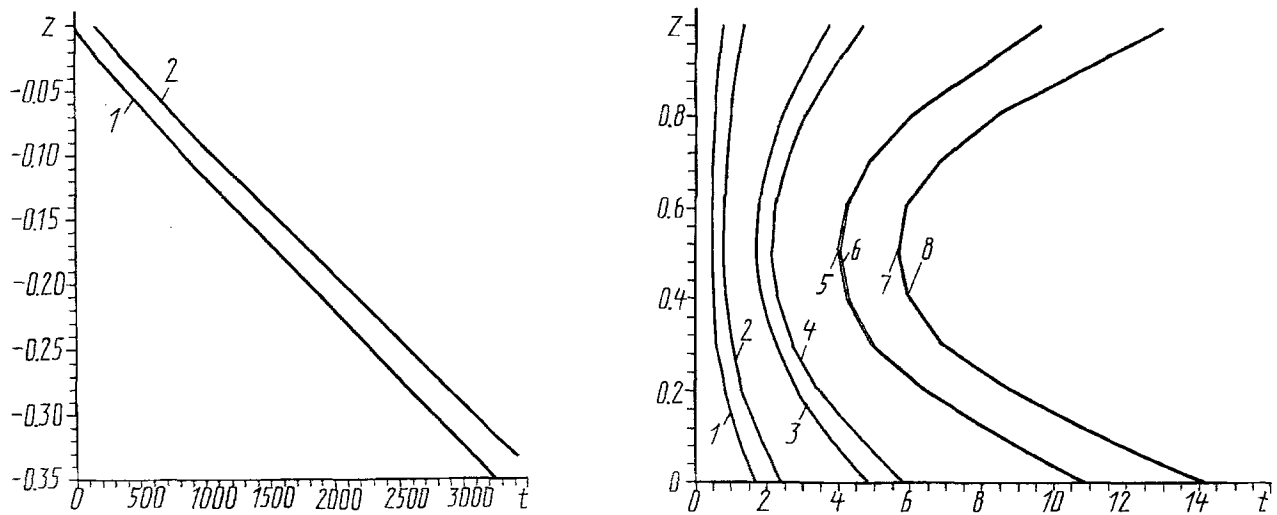


Fig. 1. Times of characteristic processes along the height of the core starting from the blocking instant of the emergency fuel assembly: 1) and 2) beginning and termination of sodium evaporation, respectively; 3) and 4) beginning and termination of melting of the fuel element shell; 5) and 6) beginning and termination of motion of the boundary between a solid phase and a two-phase zone in the fuel core; 7) and 8) beginning and termination of motion of the boundary between a two-phase zone and a liquid phase. t , sec; Z , m.

Fig. 2. Depth of sodium evaporation and of melting of a breeder material by a heat-releasing fuel mass: 1) depth of sodium evaporation, 2) melting depth of the conversion zone.

2850°C. The calculations were performed at zero latent heat of melting in order to compare their results with predictions without moving boundaries. Here, the thermophysical properties in the liquid and two-phase zones were assumed equal to those in the solid zone. Table 2 gives the calculated results as functions of the temperature drop in the two-phase zone ΔT . The temperatures at the instant the motion of the second moving boundary terminates, which are obtained from such calculations with tracing of the motion of two isotherms and from test calculations only with fixed nodes of the spatial net, are close to one another. The difference in final values of the temperature is no greater than 0.4%.

Using the TRAMS program, the emergency processes with melting of the materials of the core of a fast reactor were calculated. Here, the specific conditions of the processes considered were taken into account in special calculation modules attached to the above program.

Figure 1 shows the calculated results for melting of the most thermally stressed fuel element at the rated power with sudden blocking of the flow section for the sodium coolant in a separate fuel assembly. The radial temperature distribution and the coordinates of the moving phase boundaries in the fuel core, the steel shell, and the sodium film, surrounding the fuel element for some time after the onset of boiling, were calculated for several cross sections of the fuel element from the top to the bottom of the active section. Taking into account the significant length of the fuel element compared to its diameter, it is possible to disregard axial heat transfer from the center with maximum heat release to the ends of the fuel element, i.e., sufficient computational accuracy can be obtained using a one-dimensional program. This example contains the two indicated types of phase transitions, viz., formation of a two-phase zone in the fuel core with internal heat release distributed over its volume and classical motion of a solid-liquid interface in the steel shell. These materials and the liquid sodium film are separated into three individual calculation regions. For the sodium film, on the assumption that there is diffusion of vapor forming in it to a bubble surrounding the film a model with the phase front on the inner film surface with ideal contact with the shell is adopted. The times of sodium evaporation and of melting of the shell and the fuel core of the fuel element are obtained from calculations. It is found that, from the onset of fuel melting, the boundary between the

solid material and the two-phase zone rapidly reaches the outer boundary of the core and during most of the time of melting of the fuel core the two-phase zone occupies its entire cross section.

As an example of the calculation with two classical fronts moving concurrently in a single (as distinct from the previous example) calculation region, we chose material melting beneath the core, melted by a heat-releasing fuel mass. The first layer of such materials is a lower end shield, which is an extension of the core, with the only difference that a shield in the fuel elements contains a breeder material with a considerably smaller heat release. In calculations of the temperature distribution and the axial coordinates of the interface, this layer is regarded as a porous medium with parallel conductance of its constituents. Figure 2 depicts the interface coordinates in the shield as functions of time. One of the moving boundaries is the melting boundary of the breeder material. The fuel of the core is assumed here to expel the melting underlying material. In this case, the indicated phase boundary coincides with the surface of the calculation region. The second, from the top, moving front is the boundary of sodium evaporation moving as the fuel melt shifts a somewhat below the first front. This boundary separates a zone with a fairly high effective thermal conductivity $\lambda_{ef} = 30 \text{ W}/(\text{m} \cdot \text{deg})$ and a zone with a much lower thermal conductivity $\lambda_{ef} = 7 \text{ W}/(\text{m} \cdot \text{deg})$. The basic calculated result, viz., the time of fuel movement to the shield bottom, depends substantially on whether this factor is taken into consideration.

Thus, the devised general method of numerical solution of problems of heat conduction with phase transitions of two types provides sufficient computational accuracy. The program of computerized predictions, set up on its basis, can be utilized to calculate emergency processes with material melting in nuclear reactors.

NOTATION

r , coordinate; t , time; T , temperature; y , interface coordinate; λ , thermal conductivity; c , specific heat per unit volume; a , thermal diffusivity; T_m , melting temperature; R_m , latent heat of melting per unit volume; ΔT , temperature drop in the two-phase zone; q_v , specific heat release (per unit volume); h , spatial step of the calculation net; τ , temporal step. Subscripts and superscripts: L, liquid phase; S, solid phase; SL, two-phase zone; p , number of the interface in the calculation region; i , number of the node of the spatial net; j , number of the temporal step; N_1 and N_2 , number of the node of the spatial net located on the left or right boundary of the calculation region, respectively.

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