MORE ACCURATE DIFFERENCE SCHEMES FOR SOLVING THE HEAT-CONDUCTION EQUATION WITH BOUNDARY CONDITIONS OF THE THIRD KIND

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UDC 536.24.02

A difference analog of a boundary condition of the third kind is obtained. By integrating the heat-conduction equation numerically the surface temperature can be calculated with an error of the fourth order of smallness in the size of the space step.

1. A number of formulas have been obtained for the numerical integration of the heat-conduction equation

$$\frac{\partial t}{\partial \tau} = a\,\frac{\partial^2 t}{\partial x^2} \quad (0 \leqslant x \leqslant 2R) \tag{1}$$

by the net-point method which, according to the classification employed by Saul'ev [1], belong to the domain of higher accuracy, since the error in the solution for the inner nodes of the net is of the order $O(h^4)$. Some of these explicit type formulas are given in [1, 2].

The use of such formulas for boundary conditions of the first kind leads to an appreciable saving of calculational effort as compared with formulas which belong to the domain of optimum (ordinary) accuracy according to the same classification.

However, if boundary conditions of the third kind are replaced by difference analogs giving a lower accuracy than conditions applied at the inner nodes, the accuracy of the solution of the whole difference scheme will inevitably be diminished.

Therefore it is very necessary to investigate more accurate approximations of boundary conditions of the third kind. Samarskii [3] presents difference analogs of boundary conditions of the third kind which give an approximation of the second order of smallness in h, and schemes presented in [4] give an approximation of the order $O(l^2 + h^4)$. The difference analog of a boundary condition of the third kind of Vitácek [5] for an explicit scheme has an approximation error of the order $O(h^4)$, but the error of the solution in using this formula, i.e., the difference $t_{0,k} - \vartheta_{0,k}$ is only of the order $O(h^2)$, as was pointed out by Vitácek himself [5].

An explicit formula is presented in [6] for calculating the temperature at surface nodes, giving an accuracy of the third order of smallness in h. This explicit one-step formula has the form

$$\left(3 + \frac{\alpha h}{\lambda}\right)\vartheta_{0,k+1} = 2\vartheta_{0,k} + \vartheta_{1,k} + \frac{\alpha h}{\lambda} f(kl + l) \tag{2}$$

and assumes that the sizes of the space and time steps are related by $6al = h^2$, and therefore to calculate the temperature at internal nodes it is necessary to use also the explicit higher accuracy formula of Mikeladze and Panov

$$6\vartheta_{i,k+1} = \vartheta_{i-1,k} + 4\vartheta_{i,k} + \vartheta_{i+1,k}. \tag{3}$$

The difference scheme (2)-(3) has the merits of explicit schemes and leads to solutions with an error $O(h^3)$.

Leningrad Technological Institute of the Refrigeration Industry. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 26, No. 3, pp. 533-538, March, 1974. Original article submitted January 22, 1973.

In the present article, which is an extension of [6], we present a three-point calculational formula of the explicit type giving an accuracy of the fourth order of smallness of h.

We investigate the simplest one-dimensional case of the heat-conduction equation (1) with a boundary condition of the third kind with a variable temperature of the medium

$$\left\{ \frac{\partial t}{\partial x} \right\}_{x=0} = \frac{\alpha}{\lambda} [t(0, \tau) - f(\tau)] \tag{4}$$

using the usual rectangular net.

2. Using Taylor's theorem we can write

$$\begin{gathered} t_{0,k} = t_{0,k+1} - l \frac{\partial t_{0,k}}{\partial \tau} - \frac{l^2}{2} \frac{\partial^2 t_{0,k}}{\partial \tau^2} + O(l^3), \\ f(kl) = f(kl+l) - lf'(kl) - \frac{l^2}{2} f''(kl) + O(l^3), \\ \frac{\partial t_{0,k}}{\partial x} = \frac{t_{1,k} - t_{-1,k}}{2h} - \frac{h^2}{2} \frac{\partial^3 t_{0,k}}{\partial x^3} - \frac{h^4}{120} \frac{\partial^5 t_{0,k}}{\partial x^5} + O(h^6). \end{gathered} \tag{5}$$

We rewrite the boundary condition (4) for nodes on the left-hand boundary in the form

$$\frac{\partial t_{0,k}}{\partial x} = \frac{\alpha}{\lambda} \left[\left(1 - \frac{p}{6} \right) t_{0,k} + \frac{p}{6} t_{0,k} - \left(1 - \frac{p}{6} \right) f(kl) - \frac{p}{6} f(kl) \right], \tag{6}$$

where

$$p = \frac{h^2}{al}.$$

Then using (5)

$$\frac{t_{1,k} - t_{-1,k}}{2h} - \frac{h^2}{6} \frac{\partial^3 t_{0,k}}{\partial x^3} - \frac{h^4}{120} \frac{\partial^5 t_{0,k}}{\partial x^5} + O(h^6) = \frac{\alpha}{\lambda} \left[\left(1 - \frac{p}{6} \right) t_{0,k} \right.$$

$$\left. + \frac{p}{6} t_{0,k+1} - \frac{pl}{6} \frac{\partial t_{0,k}}{\partial \tau} - \frac{pl^2}{12} \frac{\partial^2 t_{0,k}}{\partial \tau^2} + O(l^3) - \left(1 - \frac{p}{6} \right) f(kl) - \frac{p}{6} f(kl+l) + \frac{pl}{6} f'(kl) + \frac{pl^2}{12} f''(kl) + O(l^3) \right]$$

or

$$t_{-1,k} = t_{1,k} - 2N \left(1 - \frac{p}{6} \right) t_{0,k} - \frac{Np}{3} t_{0,k+1} + 2N \left(1 - \frac{p}{6} \right) f(kl)$$

$$+ \frac{Np}{3} f(kl+l) + \left[-\frac{h^3}{3} \frac{\partial^3 t_{0,k}}{\partial x^3} + \frac{Npl}{3} \frac{\partial t_{0,k}}{\partial \tau} - \frac{Npl}{3} f'(kl) \right] + \left[-\frac{h^5}{60} \frac{\partial^5 t_{0,k}}{\partial x^5} + \frac{Npl^2}{6} \frac{\partial^2 t_{0,k}}{\partial \tau^2} - \frac{Npl^2}{6} f''(kl) \right] + O(h^7), \tag{7}$$

where

$$N = \frac{\alpha h}{\lambda}. \tag{8}$$

Since it follows from the differential equation (1) that

$$\frac{\partial^3 t}{\partial x^3} = \frac{1}{a} \frac{\partial}{\partial \tau} \left(\frac{\partial t}{\partial x} \right),$$

the first square bracket for any x in (7) takes the form

$$-\frac{h^3}{3} \left[\frac{\partial^3 t}{\partial x^3} - \frac{\alpha}{a\lambda} \left(\frac{\partial t}{\partial \tau} - f'(\tau) \right) \right] = -\frac{h^3}{3a} \frac{\partial}{\partial \tau} \left[\frac{\partial t}{\partial x} - \frac{\alpha}{\lambda} (t - f(\tau)) \right]$$

and vanishes at $x = 0$ by boundary condition (4), assuming the differentiability of the functions involved to the required order.

We show that the second square bracket in (7), which can be rewritten in the form

$$-\frac{h^5}{60} \left[\frac{\partial^5 t_{0,k}}{\partial x^5} - \frac{10\alpha}{p\lambda a^2} \left(\frac{\partial^2 t_{0,k}}{\partial \tau^2} - f''(kl) \right) \right],$$

vanishes only when $p = 10$. It follows from (1) that

$$\frac{\partial^5 t}{\partial x^5} = \frac{1}{a^2} \frac{\partial^2}{\partial \tau^2} \left(\frac{\partial t}{\partial x} \right)$$

and therefore

$$\frac{\partial^5 t}{\partial x^5} - \frac{10\alpha}{p\lambda a^2}\left(\frac{\partial^2 t}{\partial \tau^2} - f''(\tau)\right) = \frac{1}{a^2}\frac{\partial^2}{\partial \tau^2}\left[\frac{\partial t}{\partial x} - \frac{10\alpha}{p\lambda}(t - f(\tau))\right],$$

which vanishes at x = 0 only when p = 10.

Thus for p = 10 Eq. (7) can be written in the form

$$t_{-1,k} = t_{1,k} + \frac{4N}{3} t_{0,k} - \frac{10N}{3} t_{0,k+1} - \frac{4N}{3} f(kl) + \frac{10N}{3} f(kl + l) + O(h^7). \tag{9}$$

3. To calculate $t_{i,k}$ at the inner nodes it is obviously necessary to use a formula of higher accuracy which for p = 10 gives an error in the solution of the order $O(h^4)$.

We have set up the following explicit three-point formula specifically for this case

$$50t_{i,k+1} = 4t_{i,k-1} + 34t_{i,k} + 3(t_{i-1,k} + t_{i+1,k} + t_{i-1,k-1} + t_{i+1,k-1}) + R_{i,k}. \tag{10}$$

An appropriate investigation shows that the remainder $R_{i,k}$ is of the sixth order of smallness in h.

It can be shown that when the error at the nodes of the first two rows (for $\tau = 0$ and $\tau = l$) and on the boundary lines x = 0 and x = 2R is no lower than the fourth order of smallness in h, the accuracy of the solution given by the approximate formula

$$50\vartheta_{i,k+1} = 4\vartheta_{i,k-1} + 34\vartheta_{i,k} + 3(\vartheta_{i-1,k} + \vartheta_{i+1,k} + \vartheta_{i-1,k-1} + \vartheta_{i+1,k-1}), \tag{11}$$

will also be of the fourth order of smallness in h, and from the inequality

$$|t_{i,k} - \vartheta_{i,k}| < Bh^4,$$

where B does not depend on h, the approximate solution must converge to the exact solution.

The derivation is not presented here because of limitations on the length of the article. Equation (10) for i = 0, i.e., on the left-hand boundary, takes the form

$$50t_{0,k+1} = 4t_{0,k-1} + 34t_{0,k} + 3(t_{-1,k} + t_{1,k} + t_{-1,k-1} + t_{1,k-1}) + O(h^6). \tag{12}$$

We substitute $t_{-1,k}$ from (9) into the last equation and for $t_{-1,k-1}$ the value obtained from (9) by replacing k by k−1. Then

$$(25 + 5N)t_{0,k+1} = (2 + 2N)t_{0,k-1} + (17 - 3N)t_{0,k} + 3t_{1,k} + 3t_{1,k-1} - 2Nf(kl - l) + 3Nf(kl) + 5f(kl + l) + O(h^6). \tag{13}$$

Discarding the remainder in (13) we obtain the formula

$$(25 + 5N)\vartheta_{0,k+1} = (2 + 2N)\vartheta_{0,k-1} + (17 - 3N)\vartheta_{0,k} + 3\vartheta_{1,k} + 3\vartheta_{1,k-1} - 2Nf(kl - l) + 3Nf(kl) + 5f(kl + l). \tag{14}$$

Subtracting (14) from (13) we obtain

$$(25 + 5N)\xi_{0,k+1} = (2 + 2N)\xi_{0,k-1} + (17 - 3N)\xi_{0,k} + 3\xi_{1,k} + 3\xi_{1,k-1} + R_{0,k}, \tag{15}$$

where $\xi_{i,k}$ is the difference $t_{i,k} - \vartheta_{i,k}$. Denoting by δ_k a number not smaller than the maximum absolute value of ξ at all nodes on the line $\tau = kl$, and noting that the remainder $R_{0,k}$ satisfies the inequality

$$|R_{0,k}| < (25 + 5N)Alh^4$$

(A > 0 does not depend on l and h) Eq. (15) can be replaced by

$$|\xi_{0,k+1}| < \frac{5 + 2N}{25 + 5N}\delta_{k-1} + \frac{20 + 3N}{25 + 5N}\delta_k + Alh^4. \tag{16}$$

Assuming that the maximum absolute error at the nodes on the lines $\tau = 0$ and $\tau = l$ are the same ($\delta_1 = \delta_0$) and not lower than the fourth order of smallness in h, we obtain from (16) for k = 1

$$|\xi_{0,2}| < \delta_0 + Alh^4 = \delta_2.$$

Setting k = 2, 3, . . . , in (16) we have

$$|\xi_{0,3}| < \frac{5 + 2N}{25 + 5N}\delta_0 + \frac{20 + 3N}{25 + 5N}(\delta_0 + Alh^4) + Alh^4 < \delta_0 + 2Alh^4 = \delta_3,$$

$$|\xi_{0,4}| < \frac{5 + 2N}{25 + 5N}\delta_2 + \frac{20 + 3N}{25 + 5N}\delta_3 + Alh^4 < \delta_0 + 3Alh^4 = \delta_4,$$

. . . .

TABLE 1. Values of the Temperature at the Nodes

Fo	L=1	L=0,5	L=0
0,500	0,1657	0,4432	0,5493
0,250	0,2518	0,6636	0,8126
0,100	0,3649	0,8628	0,9774
0,075	0,4054	0,9053	0,9926
0,050	0,4582	0,9487	0,9993
0,025	0,5536	0,9939	1,0000
0	0,6612	1,0000	1,0000

$$|\xi_{0,k+1}| < \delta_0 + kAlh^4 = \delta_0 + \tau^* Ah^4,$$

where $\tau^* = kl$ is finite. Therefore we can write

$$|\xi_{0,k+1}| < Ch^4, \tag{17}$$

where C > 0 and does not depend on h.

From inequality (17) there follows not only the convergence of the approximate solution to the exact, i.e.,

$$\lim_{h\to 0} \vartheta_{0,k} = t_{0,k},$$

but also the proof that the accuracy of the solution obtained by Eq. (14) will be of the fourth order of smallness in h.

A formula analogous to (14) can be written for the right-hand boundary.

The simultaneous application of (11) and (14) gives the most accurate difference scheme of the explicit type known to the author.

4. We illustrate the above by an example of the cooling of a flat wall of thickness 2R having a constant initial temperature in a medium of constant temperature. By considering the symmetrical problem, for which the solution is well known [7], we can compare the approximate and exact solutions.

We rewrite the formulas in dimensionless form, introducing the conventional notation.

Equation (1) takes the form

$$\frac{\partial\theta}{\partial \mathrm{Fo}} = \frac{\partial^2\theta}{\partial L^2} \quad (-1 \leqslant L \leqslant 1), \tag{18}$$

and steps along the Fo and L axes will be $\Delta L = 2/n$; $\Delta \mathrm{Fo} = 4/pn^2$.

Since $N = 2\,\mathrm{Bi}/n$ and $\vartheta_{i,k} = t_c + (t_0 - t_c)u_{i,k}$ we have instead of Eqs. (11) and (14)

$$50u_{i,k+1} = 4u_{i,k-1} + 34u_{i,k} + 3(u_{i-1,k} + u_{i+1,k} + u_{i-1,k-1} + u_{i+1,k-1}), \tag{19}$$

$$\left(25 + \frac{10\,\mathrm{Bi}}{n}\right)u_{0,k+1} = \left(2 + \frac{4\,\mathrm{Bi}}{n}\right)u_{0,k-1} + \left(17 - \frac{6\,\mathrm{Bi}}{n}\right)u_{0,k} + 3u_{1,k} + 3u_{1,k-1}. \tag{20}$$

If, for example, we take Bi = 4 and n = 4 we obtain instead of (20)

$$35u_{0,k+1} = 6u_{0,k-1} + 11u_{0,k} + 3(u_{1,k} + u_{1,k-1}). \tag{21}$$

Since the whole thickness of the wall is divided into only four parts, the symmetry of the problem shows that it is sufficient to calculate the temperature in each layer at only three nodes: on the surface (L = 1), in the central plane (L = 0), and at L = 0.5. In this case $\Delta L = 0.5$, $\Delta \mathrm{Fo} = 4/10 \cdot 4^2 = 0.025$.

To avoid excessive errors at the beginning of the calculations we took the values of the temperature for Fo = 0.025 from the formula derived by using the infinite integral Laplace transform (for small values of Fo) cited in the monograph of Lykov [7]. In our notation it takes the form

$$\theta_{j,1} = \mathrm{erf}\,\frac{j\sqrt{p}}{2} + \exp\left(Nj + \frac{N^2}{p}\right)\mathrm{erfc}\left(\frac{j\sqrt{p}}{2} + \frac{N}{\sqrt{p}}\right)$$

$$-\mathrm{erfc}\,\frac{(n-j)\sqrt{p}}{2} + \exp\left[N(n-j) + \frac{N^2}{p}\right]\mathrm{erfc}\left[\frac{(n-j)\sqrt{p}}{2} + \frac{N}{\sqrt{p}}\right].$$

Here j denotes the number of the node counting from the surface. Having calculated $\theta_{0.2} = 0.4582$ beforehand we determine $u_{0.0} = 0.6612$ from (21). The latter value is needed to find $u_{1.2} = 0.9487$.

The beginning of the calculations is shown in Table 1.

By comparing the values obtained for Fo = 0.5 with the exact solution we estimate the relative error as 0.5%.

We note, however, that if we had taken a rougher value for $u_{0.0}$ the divergence, which is appreciable at the beginning of the calculations, would be gradually smoothed out.

NOTATION

t	is the temperature;
τ	is the time;
x	is the coordinate;
a	is the thermal diffusivity;
α	is the heat-transfer coefficient;
λ	is the thermal conductivity;
$t_c = f(\tau)$	is the ambient temperature;
n	is the number of divisions of the interval [0, 2R];
$h = 2R/n$	is the size of the space step;
l	is the size of the time step;
$t_{i,k}$	is the exact temperature at $x = ih$, $\tau = kl$;
$\vartheta_{i,k}$	is the approximate temperature at $x = ih$, $\tau = kl$;
$t_{-1,k}$	is the temperature at an auxiliary node a distance h from the surface;
$\partial t_{i,k}/\partial\tau = \{\partial t/\partial\tau\}_{x=ih, \tau=kl}$;	
$\partial^2 t_{i,k}/\partial x^2 = \{\partial^2 t/\partial x^2\}_{x=ih, \tau=kl}$;	
t_0	is the initial temperature;
$\theta = (t-t_c)/(t_0-t_c)$;	
$u_{i,k} = (\vartheta_{i,k}-t_c)/(t_0-t_c)$;	
$L = x/R$;	
$Fo = a\tau/R^2$;	
$Bi = \alpha R/\lambda$.	

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