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FINITE-DIFFERENCE METHODS FOR SIMULATING THE SOLIDIFICATION OF CASTINGS

SIMULACIJA STRJEVANJA Z METODO KONČNIH RAZLIK

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Mathematical models of casting solidification for different geometrical complexities have been developed and checked. Special emphasis is given to the numerical finite-difference methods for solving the partial differential equations for heat conduction in two- and three-dimensions, which are the basis for the simulation of solidification. In the case of three-dimensional mathematical models, the methods of Douglas and Brian are especially efficient because they are unconditionally stable and of the second order with regard to the approximation of time and space. Both methods have a two-dimensional variant and Brian´s method is identical to the implicit alternating direction method. To obtain an algorithm for the solidification with the application of implicit finite-difference methods, the system of the tri-diagonal matrix has to be solved, for which an efficient algorithm exists. In addition to the implicit methods of solving Fourier´s partial differential equation of heat conduction, also the unconditionally stable explicit finite-difference methods are used. These are the methods of partial steps, the classical method, and Saulyev's method. These methods also allow a first-order accuracy. On the basis of the quoted numerical methods for solving the partial differential equation of heat conduction, the algorithms of casting solidification of different complexity have been obtained and programmed in the computer languages ASCII FORTRAN and FORTRAN 77, and the simulation has been performed with a SPERRY 1106 computer and personal computers.

Key words: casting solidification, heat conduction method of finite differences, computer simulation

Razviti in preverjeni so bili matematični modeli za litje in strjevanje z različno geometrično kompleksnostjo. Poseben poudarek je na metodi končnih razlik za rešitev parcialnih diferencialnih enačb za prevajanje toplote v dveh in treh dimenzijah, ki so podlaga za simulacijo strjevanja. V tridimenzionalnem modelu sta posebno učinkoviti metodi po Douglasu in Brianu, ker sta nepogojno stabilni in drugega reda glede na aproksimacijo časa in prostora. Obe metodi imata tudi dvodimenzionalno varianto, Brianova metoda pa je identična z metodo implicitne alternativne diference. Za razvoj algoritma za strjevanje z metodo implicitne končne razlike je treba rešiti problem tridiagonalne matrice, za katero obstaja učinkovit algoritem. Kot dodatek implicitne metode za rešitev Fourierove parcialne diferenecialne enačbe za prevajanje toplote se uporabljajo tudi nepogojno stabilne metode končnih razlik. Med njimi so metoda delnih korakov, klasična metoda in Saulyjeva metoda, ki omogočajo, da se doseže natančnost prvega reda. Na podlagi teh numeričnih metod za rešitev parcialnih diferencialnih enačb za prevajanje toplote so bili razviti algoritmi za litje in strjevanje z različno kompleksnostjo, programirani v računalniških jezikih ASCII FORTRAN in FORTRAN 77, in izvršene simulacije z računalnikom SPERRY 1106 in na osebnem računalniku.

Ključne besede: livno strjevanje, prevajanje toplote, metoda končnih razlik, računalniška simulacije

1 INTRODUCTION

Mathematical modelling is a scientific method that provides solutions for most foundry problems that have remained unsolved for a long time, e.g., the solidification of castings. This was made possible by the rapid development of computers and numerical methods for solving partial differential equations.

The first step in establishing the mathematical models of solidification is Fourier's partial differential equation of heat conduction. In the domain of casting the equation has been solved by considering the mould geometry and the initial and boundary conditions. During the operationalization of the mathematical model the appropriate numerical methods are used: the finite-element method (FEM) [1–5] and the method of finite differences (FDM) [6–8]. The FEM is more complicated than the FDM, and it is used for castings with a complex geometry and also for curved surfaces. The FDM may be explicit and implicit [9].

For the explicit FDM the space derivative is formulated in terms of known values, whereas for the implicit FDM the space derivative is in terms of values that are yet to be computed. The explicit method allows the new value of the dependent variable to be computed essentially with repeated applications of a single formula, whereas the implicit method requires the solution of a system of simultaneous equations.

The "computational molecules" for the explicit and implicit methods are illustrated in **Figure 1**. Circles are

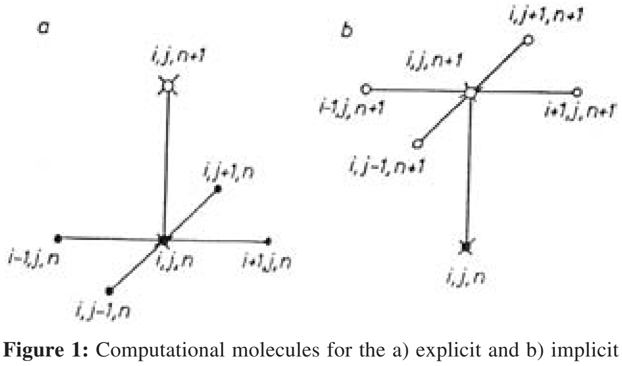

Figure 1: Computational molecules for the a) explicit and b) implicit methods
Slika 1: Računske molekule za a) eksplicitno in b) implicitno metodo

used to denote those temperatures used in formulating the space derivatives, and the crosses for those employed in the time derivative. The full circles denote values already known and the empty circles those about to be computed.

The explicit methods for solving the partial differential equation of heat conduction are usually dependent on the choice of space and time steps and are not unconditionally stable and are preferred at the operationalization of the mathematical models. However, there are some explicit methods that are unconditionally stable as well. In this work a review of the numerical methods to solve a partial differential equation of heat conduction, which has been the most frequently used during the simulation of casting solidification, is given.

2 MATHEMATICAL MODELS

The mathematical models of casting solidification consist of the partial differential equation of heat conduction with the appropriate initial and boundary conditions. The partial differential equation of heat conduction in the rectangular coordinate system has the form [10–13]:

$$\frac{\partial T}{\partial t} = a\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2}\right) \quad (1)$$

In the cylindrical coordinate system [10–13]:

$$\frac{\partial T}{\partial t} = a\left(\frac{\partial^2 T}{\partial r^2} + \frac{\partial T}{r\partial r} + \frac{\partial T}{r^2\,\partial \Theta^2} + \frac{\partial^2 T}{\partial z^2}\right) \quad (2)$$

And in the spherical coordinate system [10–13]:

$$\frac{\partial T}{\partial t} = a\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial T}{\partial r}\right) + \frac{1}{r^2 \sin\theta}\cdot\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial T}{\partial \theta}\right) + \frac{1}{r^2\sin^2\theta}\cdot\frac{\partial^2 T}{\partial \varphi^2}\right] \quad (3)$$

The initial conditions were derived on the basis of the system of thermal balance [14]:

$t = 0$ $T = T_S$

$$T_i = \frac{\rho_m C_{pm} T_L + \rho_K C_{pK} T_s + \rho_m \Delta H_f}{\rho_m C_{pm} + \rho_K C_{pk}} \quad (4)$$

The analytical solution of the partial differential equation of heat conduction for the case of the thermal contact of two semi-infinite media is [15]:

$t = 0$ $T = T_S$

$$T_{if} = T_s + \frac{T_L - T_s}{1 + \dfrac{K_K}{K_m}\sqrt{\dfrac{a_m}{a_k}}} \quad (5)$$

The boundary conditions are of the fourth kind and in a real complex system the mould-casting core-chill may be written as [15]:

$$K_m\frac{\partial T_m}{\partial n} = K_K\frac{\partial T_K}{\partial n} \quad (6)$$

$$K_m\frac{\partial T_m}{\partial n} = K_j\frac{\partial T_j}{\partial n} \quad (7)$$

$$K_m\frac{\partial T_m}{\partial n} = K_h\frac{\partial T_h}{\partial n} \quad (8)$$

$$K_k\frac{\partial T_K}{\partial n} = K_j\frac{\partial T_j}{\partial n} \quad (9)$$

The thermo-technical properties of a material that depend on the temperature [16–18] and the latent heat of crystallization are incorporated into the equation for the specific heat of the metal (the method of modified specific heat) in the following way:

$$\Delta H_f = \int_{T_s}^{T_l}(c_p^* - c_p)\,dT \quad (10)$$

3 NUMERICAL METHODS

There are two finite-difference methods for solving the three-dimensional differential equation of heat conduction in a non-stationary state: the Douglas method [6] and Brian's method [19]. The first method is a modification of the Crank-Nicolson method [6] that was proposed by Douglas:

$$\frac{1}{2}\partial_x^2(T^*_{i,j,k} + T^n_{i,j,k}) + \partial_y^2 T^n_{i,j,k} + \partial_z^2 T^n_{i,j,k} = \frac{1}{a_{i,j,k,n}}\frac{T^*_{i,j,k} - T^n_{i,j,k}}{\Delta t} \quad (11)$$

$$\frac{1}{2}\partial_x^2(T^*_{i,j,k} + T^n_{i,j,k}) + \frac{1}{2}\partial_y^2(T^{**}_{i,j,k} + T^n_{i,j,k}) + \partial_z^2 T^n_{i,j,k} = \frac{1}{a_{i,j,k,n}}\frac{T^{**}_{i,j,k} - T^n_{i,j,k}}{\Delta t} \quad (12)$$

$$\frac{1}{2}\partial_x^2(T^*_{i,j,k} + T^n_{i,j,k}) + \frac{1}{2}\partial_y^2(T^{**}_{i,j,k} + T^n_{i,j,k}) + \frac{1}{2}\partial_z^2(T^{n+1}_{i,j,k} + T^n_{i,j,k}) = \frac{1}{a_{i,j,k,n}}\frac{T^{n+1}_{i,j,k} - T^n_{i,j,k}}{\Delta t} \quad (13)$$

The second method is a modification of the Douglas-Racford method [20], and according to Brian it is the most efficient method for the numerical integration of a three-dimensional equation of heat conduction:

$$\partial_x^2 T^*_{i,j,k} + \partial_y^2 T^n_{i,j,k} + \partial_z^2 T^n_{i,j,k} = \frac{1}{a_{i,j,k,n}}\frac{T^*_{i,j,k} - T^n_{i,j,k}}{\Delta t/2} \quad (14)$$

$$\partial_x^2 T^*_{i,j,k} + \partial_y^2 T^{**}_{i,j,k} + \partial_z^2 T^n_{i,j,k} = \frac{1}{a_{i,j,k,n}}\frac{T^{**}_{i,j,k} - T^n_{i,j,k}}{\Delta t/2} \quad (15)$$

$$\partial_x^2 T^*_{i,j,k} + \partial_y^2 T^{**}_{i,j,k} + \partial_z^2 T^{***}_{i,j,k} = \frac{1}{a_{i,j,k,n}}\frac{T^{***}_{i,j,k} - T^n_{i,j,k}}{\Delta t/2} \quad (16)$$

$$\partial_x^2 T^*_{i,j,k} + \partial_y^2 T^{**}_{i,j,k} + \partial_z^2 T^{***}_{i,j,k} = \frac{1}{a_{i,j,k,n}}\frac{T^{n+1}_{i,j,k} - T^n_{i,j,k}}{\Delta t} \quad (17)$$

In practice, Brian recommended the simpler form:

$$\partial_x^2 T^*_{i,j,k} + \partial_y^2 T^n_{i,j,k} + \partial_z^2 T^n_{i,j,k} = \frac{1}{a_{i,j,k,n}}\frac{T^*_{i,j,k} - T^n_{i,j,k}}{\Delta t/2} \quad (18)$$

$$\partial_y^2 T^{**}_{i,j,k} + \partial_y^2 T^n_{i,j,k} = \frac{1}{a_{i,j,k,n}}\frac{T^{**}_{i,j,k} - T^*_{i,j,k}}{\Delta t/2} \quad (19)$$

$$\partial_z^2 T^{n+1}_{i,j,k} + \partial_z^2 T^n_{i,j,k} = \frac{1}{a_{i,j,k,n}}\frac{T^{n+1}_{i,j,k} - T^n_{i,j,k} - 2T^{**}_{i,j,k}}{\Delta t/2} \quad (20)$$

It was proved that Brian's original method can have the following form:

$$\partial_x^2 T_{i,j,k}^* + \partial_y^2 T_{i,j,k}^n + \partial_z^2 T_{i,j,k}^n = \frac{1}{a_{i,j,k,n}} \frac{T_{i,j,k}^* - T_{i,j,k}^n}{\Delta t/2} \quad (21)$$

$$\partial_x^2 T_{i,j,k}^* + \partial_y^2 T_{i,j,k}^{**} + \partial_z^2 T_{i,j,k}^n = \frac{1}{a_{i,j,k,n}} \frac{T_{i,j,k}^{**} - T_{i,j,k}^n}{\Delta t/2} \quad (22)$$

$$\partial_x^2 T_{i,j,k}^* + \partial_y^2 T_{i,j,k}^n + \partial_z^2 T_{i,j,k}^{n+1} = \frac{1}{a_{i,j,k,n}} \frac{T_{i,j,k}^{n+1} - T_{i,j,k}^{**}}{\Delta t/2} \quad (23)$$

The general solution of Brian's modified method for general points (i,j,k) and the points on the boundary surface between the mould and the metal in a rectangular coordinate system are given in Appendix A.

The methods of Douglas and Brian are unconditionally stable and converge with the discretization error $O[(\Delta t)^2 + (\Delta x)^2 + (\Delta y)^2 + (\Delta z)^2]$. Both methods have a two-dimensional option, and Brian's method is identical to the implicit alternating direction (IAD) method.

The IAD method subdivides each Δt into two half-time steps, each of duration of $\Delta t/2$. The space derivatives are approximated implicitly in the x-direction and explicitly in the y-direction over the first $\Delta t/2$; the procedure is reversed over the second $\Delta t/2$ – explicitly in the x-direction and implicitly in the y-direction. In the rectangular coordinate system it may be written as [14]:

$$\partial_x^2 T_{i,j}^{n+1/2} + \partial_y^2 T_{i,j}^n = \frac{1}{a_{i,j,n}} \frac{T_{i,j}^{n+1/2} - T_{i,j}^n}{\Delta t/2} \quad (24)$$

$$\partial_x^2 T_{i,j}^{n+1/2} + \partial_y^2 T_{i,j}^{n+1} = \frac{1}{a_{i,j,n}} \frac{T_{i,j}^{n+1} - T_{i,j}^{n+1/2}}{\Delta t/2} \quad (25)$$

And in the case of the polar coordinate system as [15]:

$$\partial_r^2 T_{i,j}^n + \frac{T_{i,j+1}^n - T_{i,j-1}^n}{2 r_j \Delta r} + \partial_z^2 T_{i,j}^{n+1/2} = \frac{1}{a_{i,j,n}} \frac{T_{i,j}^{n+1/2} - T_{i,j}^n}{\Delta t/2} \quad (26)$$

$$\partial_r^2 T_{i,j}^{n+1} + \frac{T_{i,j+1}^{n+1} - T_{i,j-1}^{n+1}}{2 r_j \Delta r} + \partial_z^2 T_{i,j}^{n+1/2} = \frac{1}{a_{i,j,n}} \frac{T_{i,j}^{n+1} - T_{i,j}^{n+1/2}}{\Delta t/2} \quad (27)$$

The implicit alternating direction method is unconditionally stable and is of second order with regard to the discretization of time and space. In parallel with the implicit alternating direction methods, the unconditionally stable explicit methods have been developed: the partial-steps method [7], the Saulyev explicit method [6,7,21–28] and the "classical" method [7]. The partial-steps method consists of two steps, which are written as:

$$\frac{T_{i,j}^{n+1/2} - T_{i,j}^n}{\Delta t} = a_{i,j,n} \partial_x^2 T_{i,j}^{n+1/2} \quad (28)$$

$$\frac{T_{i,j}^{n+1} - T_{i,j}^{n+1/2}}{\Delta t} = a_{i,j,n} \partial_y^2 T_{i,j}^{n+1} \quad (29)$$

This method is of the first order in terms of accuracy and with the approximation error $O[(\Delta t)+(\Delta x)^2+(\Delta y)^2]$.

The Saulyev method is another efficient finite-difference procedure for approximating the solution of the two-dimensional heat-conduction equation. It relies on two explicit equations, to be used in turn over successive time steps. Each equation by itself appears to be "unbalanced", but is in fact the mirror image of the other; thus the two equations may be regarded as complementary to each other. The basic computational molecules are illustrated in **Figure 2**.

From time-level n to time-level n+1 (**Figure 2a**), the derivatives are approximated as follows:

$$\frac{\partial T}{\partial t} \approx \frac{T_{i,j,n+1} - T_{i,jn}}{\Delta t} \quad (30)$$

$$\frac{\partial^2 T}{\partial x^2} \approx \frac{T_{i-1,j,n+1} - T_{i,j,n+1} - T_{i,j,n} + T_{i+1,j,n}}{(\Delta x)^2} \quad (31)$$

$$\frac{\partial^2 T}{\partial y^2} \approx \frac{T_{i,j-1,n+1} - T_{i,j,n+1} - T_{i,j,n} + T_{i,j+1,n}}{(\Delta y)^2} \quad (32)$$

This method is also of the first order in terms of accuracy. The last method for solving the two-dimensional differential equation of heat conduction is the "classical" method with the discretization error $O[(\Delta t) + (\Delta x)^2 + (\Delta y)^2]$, which may be written as:

$$\frac{T_{i,j}^{n-1} - T_{i,j}^n}{\Delta t} = a_{i,j,n} (\partial_x^2 T_{i,j}^n + \partial_y^2 T_{i,j}^n) \quad (33)$$

$$\frac{T_{i,j}^{n+1} - T_{i,j}^n}{\Delta t} = a_{i,j,n} (\partial_x^2 T_{i,j}^{n+1} + \partial_y^2 T_{i,j}^{n+1}) \quad (34)$$

Based on the quoted numerical methods for solving the partial differential equation of heat conduction, algorithms for the solidification of castings of different complexity have been obtained, as shaped-steel castings (L,T,H), as a low-carbon cast-steel gear blank, as gray iron and a cast-steel flange, a cast-steel valve housing, bars, cylinders, spheres, steel rail-wheel casting, etc. [14,15,29–46]. The algorithms are programmed in the computer languages ASCII FORTRAN and FORTRAN 77, and

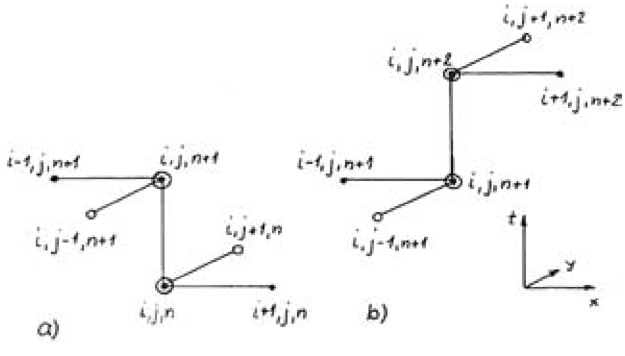

Figure 2: Computational molecules for the Saulyev method. The grid points are marked with crosses, and the full circles and empty circles are used for the time, the x-direction, and the y-direction derivatives, respectively.

Slika 2: Računske molekule za metodo po Saulyjevu. Mrežne točke označene s križci, polnimi krogi in praznimi krogi so uporabljene za čas ter x- in y-derivate.

the simulation is performed on a SPERRY 1106 computer and on personal computers.

4 CONCLUSION

Mathematical models of the casting solidification of different geometrical complexities, which are based on Fourier's differential equation of heat conduction, have been developed and investigated in this paper. To obtain satisfactory results this equation is solved by means of numerical finite-difference methods. In the case of the three-dimensional differential equation of heat conduction, two numerical methods are applied, Douglas's and Brian´s, which are unconditionally stable and are of the second order with regard to the time and space approximation. For solving the two-dimensional partial differential equation of heat conduction there are especially efficient implicit alternating direction methods, which are unconditionally stable, and the explicit methods of finite differences: the partial-step method, the "classical" method and the Saulyev method. In contrast to the implicit alternating direction methods, which are of second order with regard to the time and space approximation, the explicit methods are of first order in terms of accuracy.

List of symbols

a – thermal diffusivity
c_p – specific heat
c_p^* – specific heat in interval of solidification
ΔH_f – latent heat of fusion
K – coefficient of heat conduction
n– normal
r – coordinate
t – time
T – temperature
T^*, T^{**}- successive approximations of T at the half time-step
x,y,z – coordinate
Index:
h – chill
i – coordinate
if – temperature on the boundary surface
j – coordinate; core
k – mould
l – pouring; liquidus
m – metal
n – time step
r – coordinate
s – sand
f – fusion
x,y,z – coordinate

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Appendix A.

General solutions of Brian's modified method in a rectangular coordinate system.

When the partial differential equations of heat conduction (1), representing the solidification and cooling of steel casting in a sand mould, are approximated by means of Brian's method, the equations (21), (22) and (23) are obtained. These equations are valid for the general point (*i,j,k*) in the mould and casting. In equations (21)–(23), $a_{i,j,k,n}$ is the temperature diffusivity at the point (*i,j,k*) at temperature $T^n_{i,j,k}$. The reciprocal value of the Fourier number is:

$$Z_{i,j,k,n} = \frac{(\Delta x)^2}{a_{i,j,k,n}\Delta t} \qquad (35)$$

In the case of the equidistant net ($\Delta x = \Delta y = \Delta z$), equations (21), (22) and (23) may be written in the following form:

$$-T^*_{i-1,j,k} + 2(Z_{i,j,k,n}+1)T^*_{i,j,k} - T^*_{i+1,j,k} = T^n_{i,j-1,k} + T^n_{i,j+1,k} + T^n_{i,j,k-1} + T^n_{i,j,k+1} + 2(Z_{i,j,k,n}-2)T^n_{i,j,k} \qquad (36)$$

$$-T^{**}_{i-1,j,k} + 2(Z_{i,j,k,n}+1)T^{**}_{i,j,k} - T^{**}_{i,j,k} = T^*_{i-1,j,k} - 2T^*_{i,j,k} + T^*_{i+1,j,k} + T^n_{i,j,k-1} + T^n_{i,j,k+1} + 2(Z_{i,j,k,n}-1)T^n_{i,j,k} \qquad (37)$$

$$-T^{n+1}_{i-1,j,k} + 2(Z_{i,j,k,n}+1)T^{n+1}_{i,j,k} - T^{n+1}_{i,j,k+1} = T^*_{i-1,j,k} - 2T^*_{i,j,k} + T^*_{i+1,j,k} + T^{**}_{i,j-1,k} + 2(Z_{i,j,k,n}-1)T^{**}_{i,j,k}T^{**}_{i,j+1,k} \qquad (38)$$

Equations (21)-(23) represent the approximation for the net points in the homogeneous rectangle without boundary conditions.

In the case of the boundary interface, a perfect contact between the mould and the metal is assumed. **Figure 3** illustrates the vertical boundary surface YZ between the mould (K) and the metal (M) for an approximation of the value T^* at the point (*i,j,k*).

By means of the Taylor series, the temperatures $T^*_{i-1,j,k}$ and $T^*_{i+1,j,k}$ around $T^*_{i,j,k}$ on the vertical boundary surface are obtained:

$$T^*_{i-1,j,k} \approx T^*_{i,j,k} - \Delta x T^*_{xk} \frac{(\Delta x)^2}{2!} T^*_{xxk} \qquad (39)$$

$$T^*_{i+1,j,k} \approx T^*_{i,j,k} - \Delta x T^*_{xm} \frac{(\Delta x)^2}{2!} T^*_{xxm} \qquad (40)$$

Where $T^n_{i,j,k}$ represents the temperature derivation $\partial T^*/\partial x$ for the mould (k) in the net point (*i,j,k*). From equations (39) and (40), the derivation of the second order is expressed:

$$T^*_{xxk} = \frac{2}{(\Delta x)^2}(T^*_{i-1,j,k} - T^*_{i,j,k} + \Delta x T^*_{xk}) \qquad (41)$$

$$T^*_{xxm} = \frac{2}{(\Delta x)^2}(T^*_{i+1,j,k} - T^*_{i,j,k} + \Delta x T^*_{xm}) \qquad (42)$$

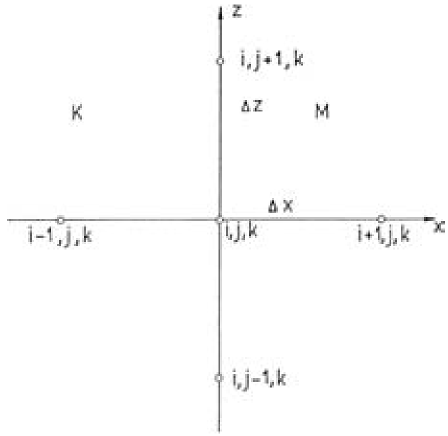

Figure 3: The vertical boundary surface YZ between the mould and the metal ($\Delta x = \Delta z$).
Slika 3: Vertikalna ločilna površina YZ med kokilo in kovino ($\Delta x = \Delta y$)

By means of Brian's method and assuming that on the boundary interface there is a continuity of heat flow:

$$K_k T^*_{xk} = K_m T^*_{xm} \qquad (43)$$

We obtain:

$$\frac{2}{(\Delta x)^2}\left[K_k(T^*_{i-1,j,k} - T^*_{i,j,k}) + K_m(T^*_{i+1,j,k} - T^*_{i,j,k})\right] + (K_k + K_m)\partial_y^2 T^n_{i,j,k} + (K_k + K_m)\partial_z^2 T^n_{i,j,k} = \left(\frac{K_k}{a_k} + \frac{K_m}{a_m}\right)\frac{T^*_{i,j,k} - T^n_{i,j,k}}{\Delta t/2} \qquad (44)$$

By dividing equation (44) with $(K_k + K_m)/(\Delta x)^2$ and with

$$Z_{i,j,k,n} = \frac{(\Delta x)^2}{\Delta t(K_k + K_m)}\left(\frac{K_k}{a_k} + \frac{K_m}{a_m}\right) \qquad (45)$$

We obtain:

$$\frac{2K_k}{K_k + K_m}T^*_{i-1,j,k} + 2(Z_{i,j,k,n}+1)Z^*_{i,j,k} - \frac{2K_m}{K_k + K_m}T^*_{i+1,j,k} = T^n_{i,j-1,k} + T^n_{i,j+1,k} + T^n_{i,j,k-1} + T^n_{i,j,k+1} + 2(Z_{i,j,k,n}-2)T^n_{i,j,k} \qquad (46)$$

By analogy, equations for the second intermediate value T^{**}(47) and the value T^{n+1} for second $\Delta t/2$ (48) are obtained:

$$-T^{**}_{i,j-1,k} + 2(Z_{i,j,k,n}+1)T^{**}_{i,j,k} - T^{**}_{i,j+1,k} = \frac{2K_k}{k_k + k_m}T^*_{i-1,j,k} - 2T^*_{i,j,k} + \frac{2K_m}{K_k + K_m}T^*_{i+1,j,k} + T^n_{i,j,k-1} + T^n_{i,j,k+1} + 2(Z_{i,j,k,n}-1)T^n_{i,j,k} \qquad (47)$$

$$-T^{n+1}_{i,j,k-1} + 2(Z_{i,j,k,n}+1)T^{n+1}_{i,j,k} - T^{n+1}_{i,j,k+1} = \frac{2K_k}{k_k + k_m}T^*_{i-1,j,k} - 2T^*_{i,j,k} + \frac{2K_m}{K_k + K_m}T^*_{i+1,j,k} + T^{**}_{i,j-1,k} + 2(Z_{i,j,k,n}-1)T^{**}_{i,j,k} + T^{**}_{i,j+1,k} \qquad (48)$$

In the same way the approximations for temperatures on the vertical XZ and the horizontal XY boundary surfaces are derived.