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MODELLING OF THE DIRECTIONAL SOLIDIFICATION OF A LEADED RED BRASS FLANGE

MODELIRANJE USMERJENEGA STRJEVANJA PRIROBNICE IZ RDEČE SVINČEVE MEDENINE

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A mathematical model and a numerical simulation of the directional solidification of a leaded red brass flange are presented. The mathematical model is based on physically realistic assumptions and it is solved by the finite-difference method, implicit alternating directions method. This method has great accuracy and is of second order with regard to the approximation of time and space. The initial conditions are an analytical solution of the heat conduction equation in the case of the contact of two semi-infinite media. The latent heat of fusion incorporated into the equation for the specific heat capacity of metal, and temperature dependent thermophysical properties of all materials in the system mould–casting–core–chill, enables us to accurately numerically represent the flange solidification, which is casting and a common example in foundry practice. The simulation of the directional solidification is a modern and scientific way of pointing to casting points in which the defect occurrence is possible, and how to prevent them using the chill.

Keywords: mathematical model, directional solidification, leaded red brass flange, graphite chill

Predstavljena sta matematični model in numerična simulacija usmerjenega strjevanja prirobnice iz rdeče svinčeve medenine. Podlaga matematičnega modela so realne fizikalne predpostavke, model pa je razvit z metodo končnih razlik, implicitno metodo z alternativno smerjo. Ta metoda je zelo natančna in je drugega reda glede na približek časa in prostora. Začetni pogoji so analitične rešitve enačbe za toplotno prevodnost za primer kontakta dveh semineskončnih medijev. Latentna talilna toplota, ki je uporabljena za specifično toplotno kapaciteto kovine in termofizikalne lastnosti vseh materialov v sistemu forma – litje – jedro – kokila omogočajo, da se numerično modelira strjevanje prirobnice, torej litje, kar je splošen primer dela v livarni. Simulacija usmerjenega strjevanja je moderna metoda, da se znanstveno opredeli mesta ulitka, kjer lahko nastajajo napake in kako te napake s kokilo preprečiti.

Ključne besede: matematični model, usmerjeno strjevanje, prirobnica, svinčeva rdeča medenina, grafitna kokila

1 INTRODUCTION

The directional solidification of castings of a given geometry may be obtained using risers or chills. Risers are reservoirs of molten metal and feed the casting in the liquid state. In the case of classical risers, only 17 pct. of the initial volume of the riser is available for the feeding of the casting 1. In contrast to risers, chills better lead away the heat and in this way speed up the solidification. Usually, they are used when the placement of risers is impossible. However, in the case of nonferrous metals this is not a rule. In this way, for example, in the investigated system of a leaded red brass flange, directional solidification is obtained using a graphite chill. With the placement of an appropriate chill, the hot spot is shifted in areas of the casting which are later machined. This is desirable because the hot spot solidifies last, and in their place the occurrence of casting defects (e.g., shrinkage cavity, porosity etc.) is possible. The investigated system is complex because it consists of a flange, a mould core and a chill, and it is shown in **Figure 1**. For a given system the mathematical model of the solidification is formulated and investigated.

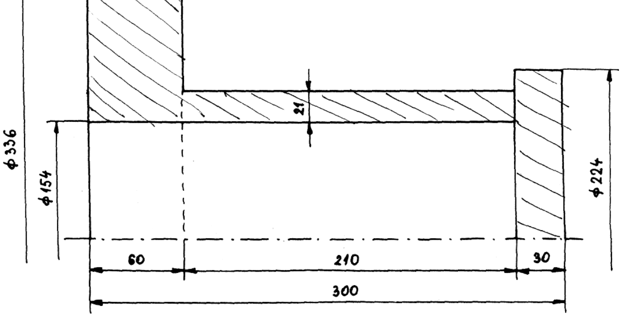

Figure 1: Flange and graphite chill with the corresponding dimensions
Slika 1: Prirobnica in grafitna kokila z dimenzijami

2 MATHEMATICAL MODEL

In the development of the mathematical model, the following partial differential equation of heat flow corresponding to the flange (**Figure 1**) [2] should be solved:

$$\frac{\partial T}{\partial t} = a\left(\frac{\partial^2 T}{\partial r^2} + \frac{1}{r}\frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial z^2}\right) \qquad (1)$$

Since for the horizontal axis of the flange symmetry $r = 0$, equation (1) should be modified according to L' Hospital's rule considering the equation:

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

Initial conditions

The mould temperature and the temperature of its outer side are equal to T_s, whereas the temperature of the metal is equal to the casting temperature T_L. The initial temperature at the mould/casting boundary interface can be obtained by solving Fourier's differential equation for heat flow through the contact area of two semi-infinite media:

$$T_i = T_s + \frac{T_L - T_s}{1+\frac{K_K}{K_m}\sqrt{\frac{a_m}{a_k}}} \tag{3}$$

The derivation of eq. (3) is given in Appendix 2.

Boundary conditions

The outer mould surface maintains a constant temperature T_s. For the contacts mould/metal, metal/core, mould/core, metal/chill, mould/chill and chill/core area there are continuous heat flows for which the boundary condition of the fourth type holds [3]:

$$K_m \frac{\partial T_m}{\partial n} = K_K \frac{\partial T_K}{\partial n} \tag{4}$$

$$K_m \frac{\partial T_m}{\partial n} = K_j \frac{\partial T_j}{\partial n} \tag{5}$$

$$K_m \frac{\partial T_m}{\partial n} = K_h \frac{\partial T_h}{\partial n} \tag{6}$$

$$K_k \frac{\partial T_K}{\partial n} = K_j \frac{\partial T_j}{\partial n} \tag{7}$$

$$K_h \frac{\partial T_h}{\partial n} = K_k \frac{\partial T_k}{\partial n} \tag{8}$$

$$K_h \frac{\partial T_h}{\partial n} = K_j \frac{\partial T_j}{\partial n} \tag{9}$$

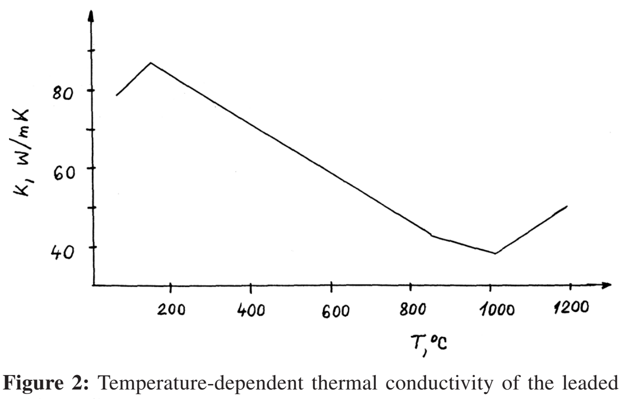

Figure 2: Temperature-dependent thermal conductivity of the leaded red brass flange

Slika 2: Odvisnost toplotne prevodnosti od temperature za prirobnico iz svinčeve rdeče medenine

Thermophysical properties of the material

It has been assumed that the thermal properties of the mould, metal, core and chill are temperature dependent [4], which is as shown in **Figures 2 to 9**.

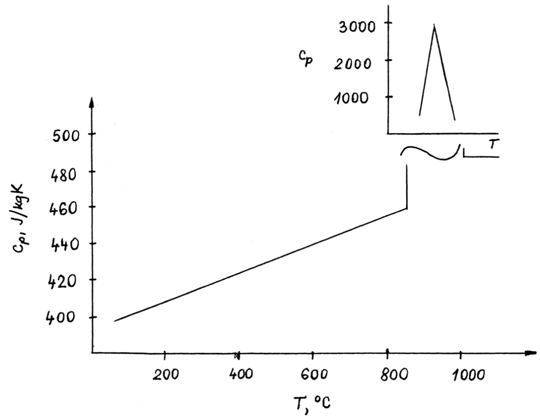

Figure 3: Temperature-dependent specific heat capacity of the leaded red brass flange

Slika 3: Odvisnost specifične toplotne kapacitete od temperature za prirobnico iz svinčeve rdeče medenine

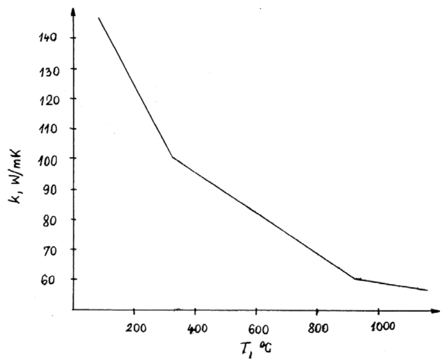

Figure 4: Temperature-dependent thermal conductivity of the graphite chill

Slika 4: Odvisnost toplotne prevodnosti od temperature za grafitno kokilo

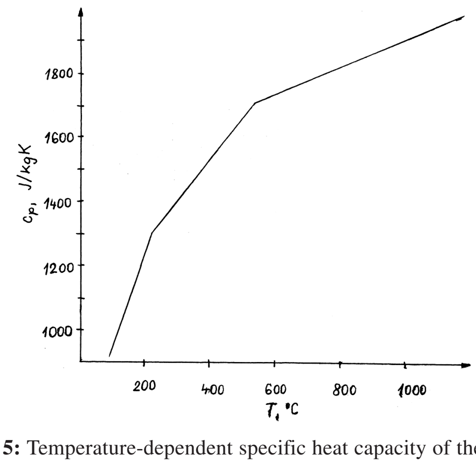

Figure 5: Temperature-dependent specific heat capacity of the graphite chill

Slika 5: Odvisnost specifične toplotne kapacitete od temperature za grafitno kokilo

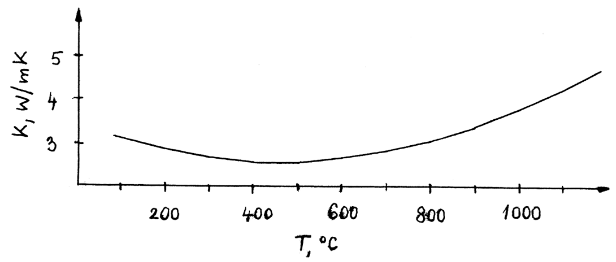

Figure 6: Temperature-dependent thermal conductivity of the mould
Slika 6: Odvisnost toplotne prevodnosti od temperature za formo

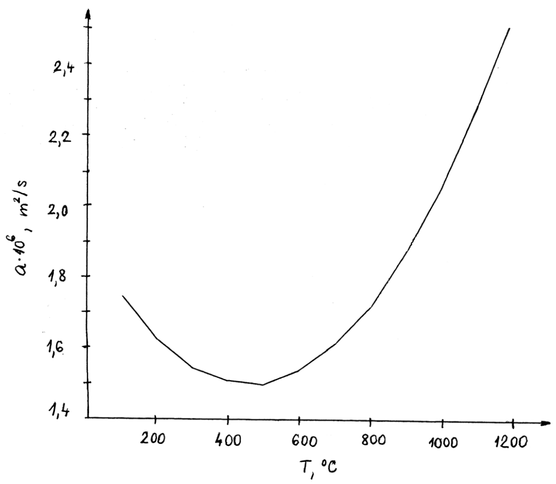

Figure 7: Temperature-dependent temperature diffusivity of the mould
Slika 7: Odvisnost toplotne difuzivnosti od temperature za formo

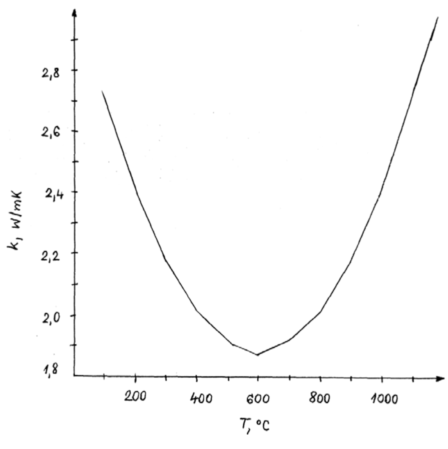

Figure 8: Temperature-dependent thermal conductivity of the core
Slika 8: Odvisnost toplotne prevodnosti od temperature za jedro

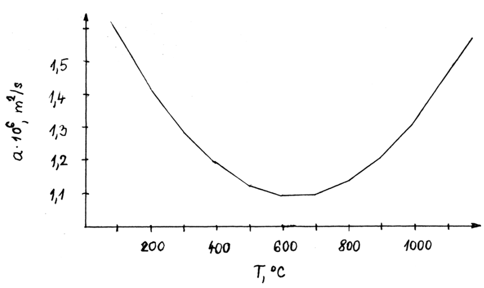

Figure 9: Temperature-dependent temperature diffusivity of the core.
Slika 9: Odvisnost toplotne difuzivnosti od temperature za jedro

3 IMPLICIT ALTERNATING DIRECTION METHOD

Differential heat-flow equations (1) and (2) with the corresponding initial and boundary conditions have been numerically solved using the implicit alternating direction method [5,6]. The method utilises the division of the time interval into two steps.

In the first half of the time interval the equation is solved implicitly for z and explicitly for the *r* direction. The procedure is reversed in the second half of the time interval.

Consequently, for the differential equation (1) and the first half of the time interval $\Delta t/2$ we have:

$$\frac{T^n_{i,j-1}-2T^n_{i,j}+T^n_{i,j+1}}{(\Delta r)^2}+\frac{T^n_{i,j+1}-T^n_{i,j-1}}{2r_j\cdot\Delta r}+ + \frac{T^n_{i-1,j}-2T^n_{i,j}+T^n_{i+1,j}}{(\Delta z)^2}=\frac{1}{a_{i,j,n}}\frac{T^*_{i,j}-T^n_{i,j}}{\Delta t/2} \tag{10}$$

Whereas for the second $\Delta t/2$ we obtain:

$$\frac{T^{n+1}_{i,j-1}-2T^{n+1}_{i,j}+T^{n+1}_{i,j+1}}{(\Delta r)^2}+\frac{T^{n+1}_{i,j+1}-T^{n+1}_{i,j-1}}{2r_j\cdot\Delta r}+ + \frac{T^*_{i-1,j}-2T^*_{i,j}+T^*_{i+1,j}}{(\Delta z)^2}=\frac{1}{a_{i,j,n}}\frac{T^{n+1}_{i,j}-T^*_{i,j}}{\Delta t/2} \tag{11}$$

The numerical solution for the differential equation (2) of the heat flow for the first $\Delta t/2$ is:

$$4\frac{T^n_{i,2}-T^n_{i,1}}{(\Delta r)^2}+\frac{T^*_{i-1,1}-2T^*_{i,1}+T^*_{i+1,1}}{(\Delta z)^2}= =\frac{1}{a_{i,1,n}}\frac{T^*_{i,1}-T^n_{i,1}}{\Delta t/2} \tag{12}$$

and for the second $\Delta t/2$:

$$4\frac{T^{n+1}_{i,2}-T^{n+1}_{i,1}}{(\Delta r)^2}+\frac{T^*_{i-1,1}-2T^*_{i,1}+T^*_{i+1,1}}{(\Delta z)^2}= =\frac{1}{a_{i,1,n}}\frac{T^{n+1}_{i,1}-T^*_{i,1}}{\Delta t/2} \tag{13}$$

The use of the implicit alternating direction method results in a system of simultaneous linear algebraic equations with the variables v_1, v_2,..., v_n of tri-diagonal form:

$$\begin{aligned}
&b_1\, v_1 + c_1\, v_2 = d_1\\
&a_2\, v_1 + b_2\, v_2 + c_2\, v_3 = d_2\\
&a_3\, v_2 + b_3\, v_3 + c_4\, v_4 = d_3\\
&\dots\dots\dots\dots\dots\dots\dots\dots\\
&a_i\, v_{i-1} + b_i\, v_i + c_i\, v_{i+1} = d_i\\
&\dots\dots\dots\dots\dots\dots\dots\dots\\
&a_{N-1}\, v_{N-2}\, b_{N-1}\, v_{N-1} + c_{N-1}\, v_N = d_{N-1}\\
&a_N v_{N-1} + b_N\, v_N = d_N
\end{aligned} \tag{14}$$

The special efficient algorithm for solving the tri-diagonal system of equations is [7]:

$$v_N = \gamma_N \tag{15}$$

$$v_i = \gamma_i - \frac{c_i v_{i+1}}{\beta_i}, \quad i = n-1, n-2, ..., 1 \tag{16}$$

where β and γ are calculated from recursive formulas

$$\beta_1 = b_1 \tag{17}$$

$$\gamma_1 = d_1/\beta_1 \tag{18}$$

$$\beta_i = b_i - \frac{a_i c_{i-1}}{\beta_{i-1}}, \quad i = 2,3,...,n \tag{19}$$

$$\gamma_i = -\frac{d_i - a_i \gamma_{i-1}}{\beta_i}, \quad i = 2,3,...,n \tag{20}$$

The tri-diagonal coefficients that give the algorithm of the flange solidification in a sand mould are presented in Appendix 3. Based on the presented algorithm a computer program was written in FORTRAN 77 and solved on an Athlon AMD 64 computer.

4 FLOW DIAGRAM

A detailed flow diagram is shown in **Figure 10a** and **10b**.

The main feature of the program is the use of two temperature matrixes, namely T and T^*. The first matrix contains the temperatures at the start and the end of the time step, and the second contains the temperature at the end of first $\Delta t/2$. Initial values are assigned to the program variables and constants. The program module TYP provides for the initial values of the temperatures, of particular net points as well as for the standardization of all the points in the mould, the casting, the chill core and their boundary interfaces. The module PRINT 1 prints out the initial temperature distribution. The system of tri-diagonal equations is then solved firstly, row by row (module ROWS), and then column by column (module COLS). The results are periodically printed over the whole geometry of the casting, the mould, the chill and the core (module PRINT 1) or over the casting geometry only (module PRINT 2) until the prescribed time t_{max}.

5 DISCUSSION

Leaded red brass (alloy C83600) has the following composition: 85 % Cu, 5 % Sn, 5 % Pb and 5 % Zn [8]. The alloy C83600 is used not only for flanges, but also for valves, pipe fittings, water pumps' meter housings and impellers, small gears, high-quality plumbing goods, statuary and plaques. These applications are possible because of its corrosion resistance, machinability, strength, bearing properties, colour and the excellent castability of the alloy.

The simulation of the solidification of the leaded red brass flange in a sand mould is carried out by the space steps Δz = 15 mm and Δr = 7 mm and the time step Δt = 5 s to t_{max} = 600 s.

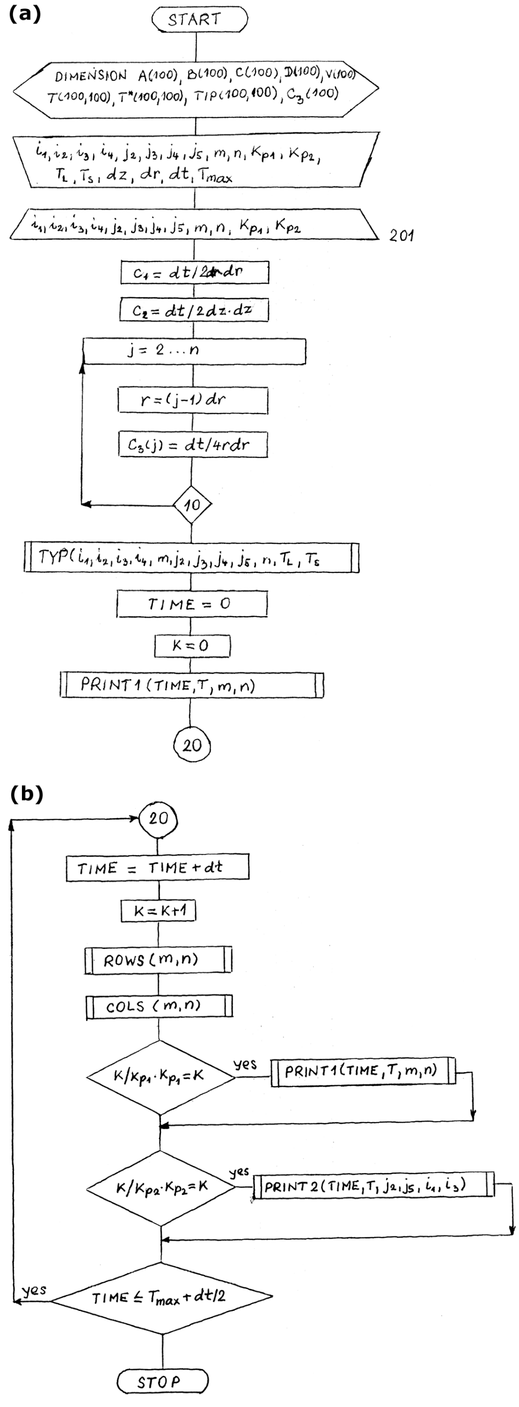

Figure 10: Flow diagram
Slika 10: Flow diagram

The casting temperature was 1180 °C and the initial temperature of the mould, the core and the chill was 25 °C. The initial temperature at the sand/casting interface was 1057 °C, on the casting/core interface it was 1013 °C, and at the casting/chill interface it was 577 °C. On the basis of successive temperature print outs for particular net points, a solidification time of 367 s was obtained.

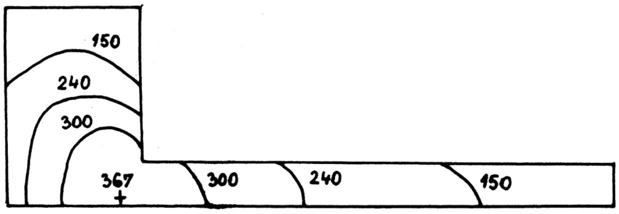

Figure 11: Progress of the isosolidus (854 °C) after (150, 240 and 300) s
Slika 11: Napredovanje izotr. (854 °C) po (150, 240 in 300) s

Using the isosolidus (854 °C) shift, as seen in **Figure 11**, it can be concluded that the potential defect site is obviously the point of the final solidification of the heat centre, i.e. in the vicinity of the core.

The accuracy of the simulation is limited, depending on the assumptions used in the mathematical model, the method of the numerical analysis and the values of thermophysical material properties used. Several assumptions were used in the elaboration of the mathematical model. The most important are as follows: the complete heat-transfer rate, a casting temperature equal to the initial temperature of the metal in the mould, and a mould/casting interface with perfect thermal contact. The first assumption restrains the analysis to the mould-casting-core-chill system with heat conduction only, i.e., partial heat flows associated with the mould and core moisture are not considered. The second assumption is the simplification introduced to avoid a complex consideration of the metal flow through the gate system and the mould cavity and the matching heat transfer. The assumption of a perfect thermal contact on the interface is acceptable because there is only a partial appearance of a gaseous clearance, and therefore in the mathematical formulation the boundary condition of the fourth kind is usually taken as valid. The partial differential equation for the heat flow is solved using a numerical method of finite difference – the implicit alternating direction method, which was chosen because of its high accuracy during the approximation of both time and space. Insufficient knowledge about the thermophysical properties of the material, especially at high temperatures, has a strong influence on the simulation of the solidification. It holds especially with respect to the thermal properties of the mould and the core material, which can be determined only experimentally. Moreover, the values for the thermal properties at higher temperatures show a considerable a dissipation.

6 CONCLUSIONS

A numerical simulation of the directional solidification of a leaded red brass flange was carried out on the basis of a suitable mathematical model. The complex model system is composed of four materials: the mould, the core, the chill and the casting of comparatively complicated geometry. The mathematical model of solidification was developed assuming thermal conduction as only heat flow in the system, which is considered as a physically real assumption. A differential equation for the heat flow suited to the flange's geometry was modified and numerically solved by the use of implicit alternating direction method. The temperature dependence of the thermophysical material's properties was taken into account. Based on the obtained algorithm a computer program written in FORTRAN 77 for an Athlon AMD 64 computer was used for the simulation of the solidification. It was determined that the complete solidification takes 367 seconds. The progress of the solidification as well as the hot spot, i.e., the site of any potential shrinkage cavity, can be determined by a shift of isosolidus.

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Appendix 1

Abbreviations used:

a –- temperature conductivity
a_i, b_i, c_i, d_i – coefficients adjoining unknowns in a tri-diagonal system of algebraic equations
c_p – specific heat capacity at constant pressure
k – thermal conductivity
n – vertical direction
r – space coordinate
t – time
T – temperature
v_i – unknown in system of simultaneous equations
z – space coordinate

Appendix 2

The following partial differential equation of heat flow with the appropriate initial and boundary conditions must be solved to derive the equation for the temperature distribution at the mould/metal interface:

$$\frac{\partial T}{\partial t}=a\frac{\partial^2 T}{\partial x^2} \tag{21}$$

$$\begin{aligned} T(x,0) &= T_s \\ T(0,t) &= T_i \\ |T(x,t)| &< M \end{aligned} \tag{22}$$

where M is a positive real constant.

The equation of heat flow should be solved for the case of the contact of two semi-infinite media. The partial differential equation (21) must be transformed into a common differential equation by the Laplace transform defined as [9]:

$$L\{T(x,t)\}=\Theta(x,s)=\int_0^\infty \mathrm{e}^{-st}\,T(x,t)\mathrm{d}t \tag{23}$$

Equation (21) in the Laplace region has the from:

$$\frac{d^2\Theta}{dx^2}-\frac{1}{a}s\Theta=-\frac{1}{a}T_s \tag{24}$$

The solution of (24) has the form:

$$\Theta(x,s)=c_1(s)\exp(x\sqrt{s/a})+c_2(s)\exp(-x\sqrt{s/a})+\frac{T_s}{s} \tag{25}$$

Because of temperature limitations, $|T(x,t)| < M$, $c_1 = 0$ for $x \to \infty$, i.e.

$$\Theta(x,s)=c_2\exp(-x\sqrt{s/a})+\frac{T_s}{s} \tag{26}$$

For the boundary condition $T(0,t) = T_i$, i.e.

$$\Theta(0,s)=c_2+\frac{T_s}{s}=\frac{T_i}{s},\quad c_2=\frac{1}{s}(T_1-T_s)$$

The final result in the Laplace region is:

$$\Theta(x,s)=\frac{T_i-T_s}{s}\exp(-x\sqrt{s/a})+\frac{T_s}{s} \tag{27}$$

By passing from the Laplace region into real space, we have:

$$T(x,t)=(T_1-T_s)\mathrm{erfc}\left(\frac{x}{2\sqrt{at}}\right)+T_s \tag{28}$$

respectively

$$\frac{(T-T_i)}{(T_s-T_i)}=\mathrm{erf}\left(\frac{x}{2\sqrt{at}}\right) \tag{29}$$

where the error function is defined as [10]:

$$\mathrm{erf}\,(t)=\frac{2}{\sqrt{\pi}}\int_0^t \mathrm{e}^{-u^2}\,\mathrm{d}u \tag{30}$$

The temperature gradient along the x-axis is:

$$\frac{\partial T}{\partial x}=\frac{T_s-T_i}{\sqrt{\pi a t}}\exp(-x^2/4at) \tag{31}$$

respectively

$$\left(\frac{\partial T}{\partial x}\right)_{x=0}=\frac{T_s-T_i}{\sqrt{\pi a t}} \tag{32}$$

Two semi-infinite media (mould and metal) are in interfacial contact and the boundary condition of the fourth kind is valid:

$$-k_k\left(\frac{\partial T_k}{\partial x}\right)_{x=0}=-k_m\left(\frac{\partial T_m}{\partial x}\right)_{x=0} \tag{33}$$

By including the proper temperature gradients:

$$k_k\frac{T_i-T_s}{\sqrt{\pi a_k t}}=k_m\frac{T_L-T_i}{\sqrt{\pi a_m t}} \tag{34}$$

Finally, the initial temperature distribution on the boundary mould/metal surface is obtained:

$$T_i=T_s+\frac{T_L-T_s}{1+\frac{K_K}{K_m}\sqrt{\frac{a_m}{a_k}}} \tag{35}$$

Appendix 3

The constants, which in tri-diagonal coefficients, are:

$$p_1=\frac{a\Delta t}{2(\Delta r)^2}$$

$$p_2=\frac{a\Delta t}{4r_j\cdot\Delta r}$$

$$p_3 = p_1 - p_2$$

$$p_4 = p_1 + p_2$$

$$p_5=\frac{\Delta t(k_\mathrm{A}+k_\mathrm{B})}{2c(\Delta r)^2}$$

$$p_6=\frac{\Delta t(k_\mathrm{A}+k_\mathrm{B})}{4cr_j\cdot\Delta r}$$

$$c=\frac{k_\mathrm{A}}{a_\mathrm{A}}+\frac{k_\mathrm{B}}{a_\mathrm{B}}$$

$$q_1=\frac{a\Delta t}{2(\Delta z)^2}$$

$$q_2=\frac{k_\mathrm{A}\Delta t}{c(\Delta z)^2}$$

$$q_3=\frac{k_\mathrm{B}\Delta t}{c(\Delta z)^2}$$

$$q_4=\frac{\Delta t(k_\mathrm{A}+k_\mathrm{B})}{2c(\Delta z)^2}$$

$$q_5=\frac{k_\mathrm{A}\Delta t}{c(\Delta r)^2}$$

$$q_6=\frac{k_\mathrm{B}\Delta t}{c(\Delta r)^2}$$

Tri-diagonal coefficients

1. Point (i,j) in the mould, metal core or chill – first $\Delta t/2$:

$$a_i = c_i = -q_1$$
$$b_i = 1 + 2q_1 \tag{36}$$
$$d_i = p_3 T^n_{i,j-1} + (1-2p_1)T^n_{i,j} + p_4 T^n_{i,j+1}$$

– second $\Delta t/2$:

$$a_j = -p_3$$
$$b_j = 1 + 2p_1$$
$$c_j = -p_4 \tag{37}$$
$$d_j = q_1 T^*_{i-1,j} + (1-2q_1)T^*_{i,j} + q_1 T^*_{i+1,j}$$

2. Point (i,j) on the boundary surface parallel to the r axis separating the material A (left) and B (right)

– first $\Delta t/2$:

$$a_i = -q_2$$
$$b_i = 1 + q_2 + q_3$$
$$c_i = -q_3 \tag{38}$$
$$d_i = (p_5 - p_6)T^n_{i,j-1} + (1-2p_5)T^n_{i,j} + (p_5 + p_6)T^n_{i,j+1}$$

– second $\Delta t/2$:

$$a_j = -(p_5 - p_6)$$
$$b_j = 1 + 2p_5$$
$$c_j = -(p_5 - p_6) \tag{39}$$
$$d_j = q_2 T^*_{i-1,j} + (1 - q_2 - q_3)T^*_{i,j} + q_3 T^*_{i+1,j}$$

3. Point (i,j) on the boundary surface parallel to the z axis separating the material A (down) and B (up).

– first $\Delta t/2$:

$$a_i = c_i = -q_4$$
$$b_i = 1 + 2q_4 \tag{40}$$
$$d_i = (q_5 - q_6)T^n_{i,j-1} + (1-2p_5)T^n_{i,j} + (q_5 + q_6)T^n_{i,j+1}$$

– second $\Delta t/2$:

$$a_j = p_6 - q_5$$
$$b_j = 1 + p_5$$
$$c_j = -(q_5 - p_6) \tag{41}$$
$$d_j = q_4 T^*_{i-1,j} + (1-2q_4)T^*_{i,j} + q_4 T^*_{i+1,j}$$

4. Point $(i,1)$ out of the boundary surface

– first $\Delta t/2$:

$$a_i = c_i = -q_1$$
$$b_i = 1 + 2q_1 \tag{42}$$
$$d_i = (1-4p_1)T^n_{i,1} + 4p_1 T^n_{i,2}$$

– second $\Delta t/2$:

$$b_j = 1 + 4p_1$$
$$c_j = 4p_1 \tag{43}$$
$$d_j = q_1 T^*_{i-1,1} + (1-2q_1)T^*_{i,1} + q_1 T^*_{i+1,1}$$

5. Point $(i,1)$ on the boundary surface, which separates the material A (left) and B (right)

– first $\Delta t/2$:

$$a_i = -q_2$$
$$b_i = 2q_4 + 1$$
$$c_i = -q_3 \tag{44}$$
$$d_i = (1-4p_5)T^n_{i,1} + 4p_5 T^n_{i,2}$$

– second $\Delta t/2$:

$$b_j = 4p_5 + 1$$
$$c_j = -4p_5 \tag{45}$$
$$d_j = q_2 T^*_{i-1,1} + (1-2q_4)T^*_{i,1} + q_3 T^*_{i+1,1}$$