# Kompjutorska simulacija skrućivanja odljevaka kompleksne geometrije

# Computer Simulation of Solidification of Complex Geometry Castings

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## 1. UVOD

Pri proizvodnji odljevaka složene geometrije od velike su pomoći modeli kojima se simulira njihovo skrućivanja jer je već za kompjutorskim terminalom moguće odrediti tok njihova skrućivanja, vrijeme skrućivanja, mjesta moguće pojave defekta u odljevcima, te utjecati na njihov dizajn kako bi se proizvedli zdravi odljevci. Međutim, raznolikost i kompleksnost oblika odljevaka umnogome otežavaju simulaciju skrućivanja jer je potrebno primijeniti kompleksan matematički aparat da bi se proces opisao matematičkim modelom koji uz osnovnu diferencijalnu jednadžbu provođenja topline sadrži početne i granične uvjete. Diferencijalna jednadžba rješava se numerički primjenom metode konačne razlike ili konačnog elementa. Metoda konačne razlike može biti eksplicitna i implicitna a po svojoj matematičkoj formulaciji nešto je jednostavnija od metode konačnog elementa, što je uvjetovalo da se ta metoda prije koristila pri rješavanju krućivanja odljevaka. Ne ulazeći u prednosti ili nedostatke navedenih metoda općenito je prihvaćeno da se kod modeliranja skrućivanja odljevaka manje složene geometrije za numeričko rješavanje parcijalne diferencijalne jednadžbe koristi metoda konačne razlike. Primjer odljevka relativno složene geometrije predstavlja kućište ventila **(slika 1)**, čiji matematički model skrućivanja sadrži numeričko rješenje parcijalne diferencijalne jednadžbe implicitnom metodom promjenljivog smjera.

## 2. MATEMATIČKI MODEL

Pri operacionalizaciji matematičkog modela potrebno je riješiti parcijalnu diferencijalnu jednadžbu provođenja topline koja odgovara geometrijskom uzoru kućišta ventila (slika 1)[(1)]:

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

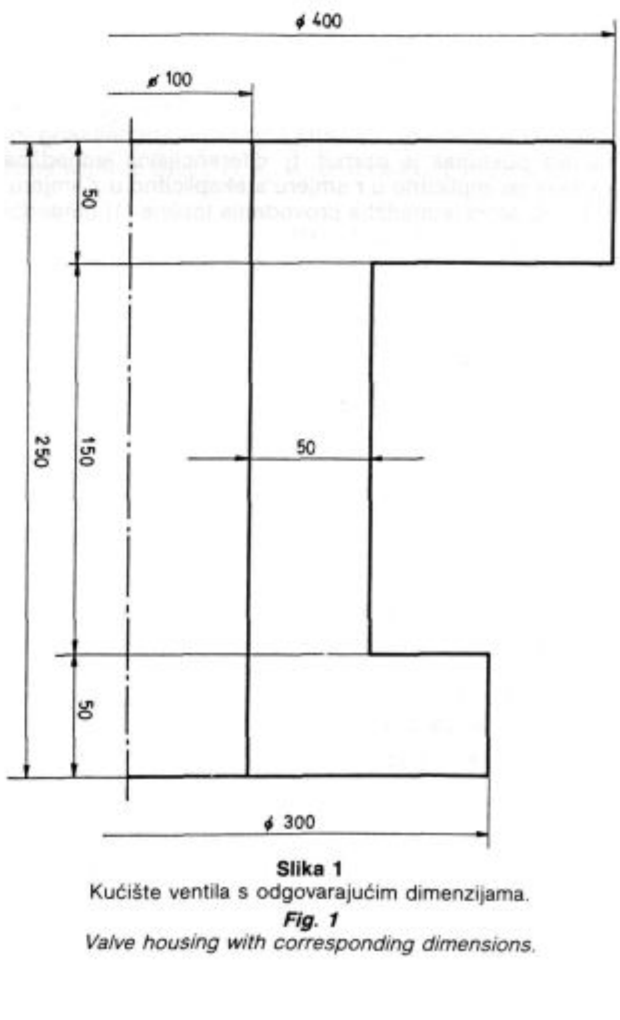
Kako u horizontalnoj osi simetrije kućišta ventila vrijedi da je $r = 0$, jednadžbu (1) potrebno je modificirati pomoću L'Hospitalovog pravila nakon čega se dobije diferencijalna jednadžba slijedećeg oblika:

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

**Početni uvjeti.** Temperatura kalupa i njegove vanjske strane jednaka je $T_s$, dok je temperatura metala u kalupu jednaka temperaturi lijevanja $T_L$. Početna temperatura na

## *1. INTRODUCTION*

*Computer simulation of solidification is very helpful for castings of complex geometry since it enables reliable determination of the course of solidification, the time required for complete solidification and the points of potential casting defects. The simulation can also contribute to improve casting design in order to assure sound castings. However, the simulation is very difficult in the case of complex geometrical shape because it requires the elaboration of a sophisticated mathematical model which beside basic differential equation of heat flow must include initial and boundary conditions also.*




**Slika 1**
Kućište ventila s odgovarajućim dimenzijama.
***Fig. 1***
*Valve housing with corresponding dimensions.*

*[1] Institut za metalurgiju, Sisak

graničnoj plohi između odljevka i kalupa dobije se rješavanjem Fourierove diferencijalne jednadžbe provođenja topline u slučaju kontakta dvaju polubeskonačnih medija:

$$T_1 = T_s + \frac{T_L - T_s}{1 + \frac{k_k}{k_m}\sqrt{\frac{a_m}{a_k}}} \tag{3}$$

Izvod jednadžbe (3) dan je u Dodatku 2.

**Granični uvjeti.** Vanjska strana kalupa drži se pri konstantnoj temperaturi $T_s$. Na dodirnoj plohi kalup-metal, metal-jezgra i kalup-jezgra postoji kontinuitet toplinskog toka odnosno vrijedi granični uvjet četvrte vrste:

$$k_m \frac{\delta T_m}{\delta n} = k_k \frac{\delta T_k}{\delta n} \tag{4}$$

$$k_m \frac{\delta T_m}{\delta n} = k_j \frac{\delta T_j}{\delta n} \tag{5}$$

$$k_k \frac{\delta T_k}{\delta n} = k_j \frac{\delta T_j}{\delta n} \tag{6}$$

**Toplofizička svojstva materijala.** Pri simulaciji skrućivanja kućišta ventila toplinska svojstva kalupa, metala i jezgre uzeta su kao funkcija temperature[2] (Dodatak 3).

## 3. IMPLICITNA METODA PROMJENLJIVOG SMJERA

Diferencijalna jednadžba provođenja topline (1) odnosno (2) s odgovarajućim početnim i graničnim uvjetima riješena je numeričkom metodom konačne razlike - implicitnom metodom promjenljivog smjera[3]. Metoda se sastoji u tome da se vremenski interval podijeli na dva koraka. U prvoj polovini vremenskog intervala diferencijalna jednadžba rješava se implicitno u z smjeru, a eksplicitno u r smjeru. Za drugu polovinu vremenskog intervala postupak je obrnut, tj. diferencijalna jednadžba rješava se implicitno u r smjeru a eksplicitno u z smjeru. Diferencijalna jednadžba provođenja topline (1) numerički se rješava na slijedeći način:

— za prvi $\Delta t/2$ vrijedi

$$\frac{T^n_{i,j-1} - 2T^n_{i,j} + T^n_{i,j+1}}{(\Delta r)^2} + \frac{T^n_{i,j+1} - T^n_{i,j-1}}{2 r_j \Delta r} + \frac{T^{n+1/2}_{i-1,j} - 2T^{n+1/2}_{i,j} + T^{n+1/2}_{i+1,j}}{(\Delta z)^2} = \frac{1}{a_{i,j,n}} \frac{T^{n+1/2}_{i,j} - T^n_{i,j}}{\Delta t/2} \tag{7}$$

— za drugi $\Delta t/2$ vrijedi

$$\frac{T^{n+1}_{i,j-1} - 2T^{n+1}_{i,j} + T^{n+1}_{i,j+1}}{(\Delta r)^2} + \frac{T^{n+1}_{i,j+1} - T^{n+1}_{i,j-1}}{2 r_j \Delta r} + \frac{T^{n+1/2}_{i-1,j} - 2T^{n+1/2}_{i,j} + T^{n+1/2}_{i+1,j}}{(\Delta z)^2} = \frac{1}{a_{i,j,n}} \frac{T^{n+1/2}_{i,j} - T^{n+1/2}_{i,j}}{\Delta t/2} \tag{8}$$

Diferencijalna jednadžba provođenja topline (2) numerički se rješava na slijedeći način:

— za prvi $\Delta t/2$ vrijedi

$$2\frac{2T^n_{i,2} - 2T^n_{i,1}}{(\Delta r)^2} + \frac{T^{n+1/2}_{i-1,1} - 2T^{n+1/2}_{i,1} + T^{n+1/2}_{i+1,1}}{(\Delta z)^2} = \frac{1}{a_{i,1,n}} \frac{T^{n+1/2}_{i,1} - T^n_{i,1}}{\Delta t/2} \tag{9}$$

*Differential equation can be solved numerically by the method of finite difference or finite elements. The method of finite difference can be explicit or implicit. In respect to mathematical formulation it is more simple than the method of finite element therefore it has been used more frequently for the solving of solidification problem. Without consideration of shortages and advantages of the both methods it has generally been accepted that for modelling of solidification of casting with less complex shape the method of finite difference is more suitable for numerical solution of corresponding partial differential equation. Valve housing* ***(Fig. 1)*** *is an example of a casting with comparatively complex geometry. Mathematical model of its solidification contains numerical solution of partial differential equation by implicit method of variable direction.*

## 2. MATHEMATICAL MODEL

*In the elaboration of mathematical model the following partial differential equation of heat flow corresponding to valve housing (Fig. 1)[1] should be solved:*

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

*Since for horizontal axis of valve housing symmetry $r=0$ equation (1) should be modified according to L'Hospital's rule which results in the equation:*

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

*Initial conditions. Mold temperature and temperature of its outer side is equal to $T_s$ whereas the temperature of metal is equal to casting temperature $T_L$. Initial temperature at the mold/casting boundary interface can be obtained by solving Fourier's differential equation for heat flow through the contact area of two semiinfinite medias:*

$$T_1 = T_s + \frac{T_L - T_s}{1 + \frac{k_k}{k_m}\sqrt{\frac{a_m}{a_k}}} \tag{3}$$

*Derivation of eq. (3) is given in Appendix 2.*

*Boundary conditions. Outer mold surface maintains constant temperature $T_S$. On contact mold/metal, metal/core and mold/core area there is a continuous heat flow for which boundary condition of the fourth sort holds:*

$$k_m \frac{\delta T_m}{\delta n} = k_k \frac{\delta T_k}{\delta n} \tag{4}$$

$$k_m \frac{\delta T_m}{\delta n} = k_j \frac{\delta T_j}{\delta n} \tag{5}$$

$$k_k \frac{\delta T_k}{\delta n} = k_j \frac{\delta T_j}{\delta n} \tag{6}$$

*Thermophysical properties of material. It has been asummed that thermal properties of mold, metal and core are temperature dependent[2]. (Appendix 3).*

## 3. IMPLICIT METHOD OF VARIABLE DIRECTION

*Differential heat flow equations (1) and (2) with corresponding initial and boundary conditions have been numerically solved by implicit method of variable direction[3]. The method utilize division of time interval into two steps. In the first half of time interval the equation is solved implicitly for z and explicitly for r direction. The procedure is reversed in the second half of time interval.*

— za drugi $\Delta t/2$ vrijedi

$$2\frac{2T_{i,2}^{n+1}-2T_{i,1}^{n+1}}{(\Delta r)^2}+\frac{T_{i-1,1}^{n+1/2}-2T_{i,1}^{n+1/2}+T_{i+1,1}^{n+1/2}}{(\Delta z)^2}=$$

$$=\frac{1}{a_{i,1,n}}\frac{T_{i,1}^{n+1}-T_{1,1}^{n+1/2}}{\Delta t/2} \qquad (10)$$

Primjenom implicitne metode promjenljivog smjera dobije se sistem simultanih linearnih algebarskih jednadžbi, čije su nepoznanice $v_1, v_2, \ldots, v_n$, a koje imaju tridijagonalni oblik:

$$\begin{array}{ll}
b_1v_1+c_1v_2 & =d_1\\
a_2v_1+b_2v_2+c_2v_3 & =d_2\\
\quad a_3v_2+b_3v_3+c_3v_4 & =d_3\\
\quad\ldots\ldots & \\
\quad\quad a_iv_{i-1}+b_iv_i+c_iv_{i+1} & =d_i \qquad (11)\\
\quad\quad\quad\ldots\ldots & \\
\quad\quad\quad a_{N-1}v_{N-2}+b_{N-1}v_{N-1}+c_{N-1}v_N & =d_{N-1}\\
\quad\quad\quad\quad a_Nv_{N-1}+b_Nv_N & =d_N
\end{array}$$

Posebno efikasan algoritam za rješavanje tridijagonalnog sistema jednadžbi je:

$$v_N=\gamma_N \qquad (12)$$

$$v_i=\gamma_i-\frac{c_i\,v_{i+1}}{\beta_i},\ i=N-1,\ N-2,\ \ldots,\ 1 \qquad (13)$$

gdje se $\beta$ i $\gamma$ računaju iz rekurzivnih formula

$$\beta_1=b_1 \qquad (14)$$

$$\gamma_1=d_1/\beta_1 \qquad (15)$$

$$\beta_i=b_i-\frac{a_i}{ci-1}\beta_{i-1},\ =2,3,\ldots,N \qquad (16)$$

$$\gamma_i=\frac{d_i-a_1\gamma_{i-1}}{\beta_i},\ i=2,3,\ldots,N \qquad (17)$$

U Dodatku 4 navedeni su tridijagonalni koeficijenti koji daju algoritam procesa skrućivanja kućišta ventila u pješčanom kalupu.

## 4. DIJAGRAM TOKA

Na temelju prikazanog algoritma napisan je program u programskom jeziku ASCII FORTRAN koji je riješen na računalu SPERRY 1100. Detaljan dijagram toka prikazan je na **slici 2**. Osnovna karakteristika programa je da se koriste dvije matrice temperatura T i T*. Prva matrica sadrži temperature na početku i kraju vremenskog koraka, a druga matrica sadrži temperature na kraju prvog $\Delta t/2$. Na početku programa pridaju se početne vrijednosti pojedinim varijablama i konstantama. Potprogramom TYP pridaju se početne vrijednosti temperature pojedinim mrežnim točkama, a također se tipiziraju sve točke u kalupu, odljevku, jezgri i na njihovim međusobnim granicama. Nakon ispisa početne temperature raspodjele pomoću potprograma ISPIS1, sistem algevarskih tridijagonalnih jednadžbi rješava se prvo redak po redak (potprogram RED), a zatim stupac po stupac (potprogram STUP). Rezultati se periodički ispisuju po cijeloj geometriji odljevka, kalupa i jezgre (potprogram ISPIS1) ili samo po geometriji odljevka (potprogram ISPIS2) do unaprijed zadanog vremena $t_{max}$.

## 5. DISKUSIJA REZULTATA

Simulacija skrućivanja ventila od čeličnog lijeva s oko 0,25% C u pješčanom kalupu provedena je uz prostorni korak $\Delta z=\Delta r=1$ cm i vremenski korak $\Delta t=10$ s do vre-

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

$$\frac{T_{i,j-1}^{n}-2T_{i,j}^{n}+T_{i,j+1}^{n}}{(\Delta r)^2}+\frac{T_{i,j+1}^{n}-T_{i,j-1}^{n}}{2r_j\,\Delta r+}$$

$$+\frac{T_{i-1,j}^{n+1/2}-2T_{i,j}^{n+1/2}+T_{i+1,j}^{n+1/2}}{(\Delta z)^2}=\frac{1}{a_{i,j,n}}\frac{T_{i,j}^{n+1/2}-T_{i,j}^{n}}{\Delta t/2} \qquad (7)$$

*Whereas for the second t/2 we obtain:*

$$\frac{T_{i,j-1}^{n+1}-2T_{i,j}^{n+1}+T_{i,j+1}^{n+1}}{(\Delta r)^2}+\frac{T_{i,j+1}^{n+1}-T_{i,j-1}^{n+1}}{2r_j\Delta r}+$$

$$+\frac{T_{i-1,j}^{n+1/2}-2T_{i,j}^{n+1/2}+T_{i+1,j}^{n+1/2}}{(\Delta z)^2}=\frac{1}{a_{i,j,n}}\frac{T_{i,j}^{n+1/2}-T_{i,j}^{n+1/2}}{\Delta t/2} \qquad (8)$$

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

$$2\frac{2T_{i,2}^{n}-2T_{i,1}^{n}}{(\Delta r)^2}+\frac{T_{i-1,1}^{n+1/2}-2T_{i,1}^{n+1/2}+T_{i+1,1}^{n+1/2}}{(\Delta z)^2}=$$

$$=\frac{1}{a_{i,1,n}}\frac{T_{i,1}^{n+1/2}-T_{1,1}^{n}}{\Delta t/2} \qquad (9)$$

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

$$2\frac{2T_{i,2}^{n+1}-2T_{i,1}^{n+1}}{(\Delta r)^2}+\frac{T_{i-1,1}^{n+1/2}-2T_{i,1}^{n+1/2}+T_{i+1,1}^{n+1/2}}{(\Delta z)^2}=$$

$$=\frac{1}{a_{i,1,n}}\frac{T_{i,1}^{n+1}-T_{1,1}^{n+1/2}}{\Delta t/2} \qquad (10)$$

*The use of implicit method of variable direction results in a system of simultaneous linear algebraic equations with variables $v_1, v_2 \ldots v_n$ of tridiagonal form:*

$$\begin{array}{ll}
b_1v_1+c_1v_2 & =d_1\\
a_2v_1+b_2v_2+c_2v_3 & =d_2\\
\quad a_3v_2+b_3v_3+c_3v_4 & =d_3\\
\quad\ldots\ldots & \\
\quad\quad a_iv_{i-1}+b_iv_i+c_iv_{i+1} & =d_i \qquad (11)\\
\quad\quad\quad\ldots\ldots & \\
\quad\quad\quad a_{N-1}v_{N-2}+b_{N-1}v_{N-1}+c_{N-1}v_N & =d_{N-1}\\
\quad\quad\quad\quad a_Nv_{N-1}+b_Nv_N & =d_N
\end{array}$$

*Specially efficient algoritm for the solving of tridiagonal system of equations is:*

$$v_N=\gamma_N \qquad (12)$$

$$v_i=\gamma_i-\frac{c_i\,v_{i+1}}{\beta_i},\ i=N-1,\ N-2,\ \ldots,\ 1 \qquad (13)$$

*where $\beta$ and $\delta$ are calculated from recursive formulas*

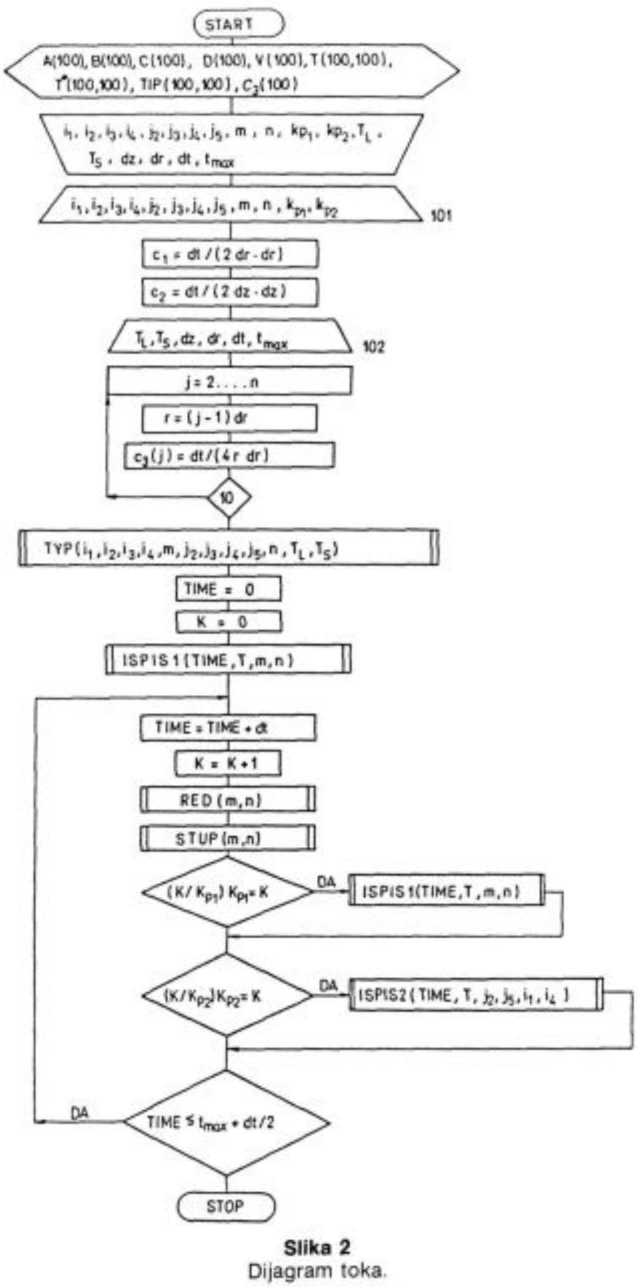
$$\beta_1=b_1 \qquad (14)$$

$$\gamma_1=d_1/\beta_1 \qquad (15)$$

$$\beta_i=b_i-\frac{a_i}{ci-1}\beta_{i-1},\ =2,3,\ldots,N \qquad (16)$$

$$\gamma_i=\frac{d_i-a_1\gamma_{i-1}}{\beta_i},\ i=2,3,\ldots,N \qquad (17)$$

*Tridiagonal coefficients which give algorithm of valve housing solidification in sand mould are presented in Appendix 4.*




**Slika 2**
Dijagram toka.
***Fig. 2***
*Flow diagram.*

mena $t_{max} = 200$ s. Temperatura lijevanja bila je 1580°C a početna temperatura kalupa i jezgre 25°C. Na temelju sukcesivnih temperaturnih ispisa za pojedine mrežne točke dobije se vrijeme skrućivanja desnog toplinskog centra od 136 s i lijevog toplinskog centra 181 s, što ujedno predstavlja vrijeme skrućivanja cijelog odljevka. Na temelju pomicanja izosolidusa (**slika 3**) može se zaključiti da su mjesta moguće pojave defekta (lunkera) upravo mjesta gdje završava skrućivanje toplinskih centara, odnosno u blizini unutarnjeg ugla odljevka. Iz **slike 3** uočava se da jezgra bolje odvodi toplinu od kalupnog materijala jer su izosolidusi pomaknuti više prema periferiji odljevka.

Točnost simulacije skrućivanja čeličnog ventila u pješčanom kalupu ograničena je s tri aspekta: predpostavkama uvedenim pri definiranju matematičkog mode-

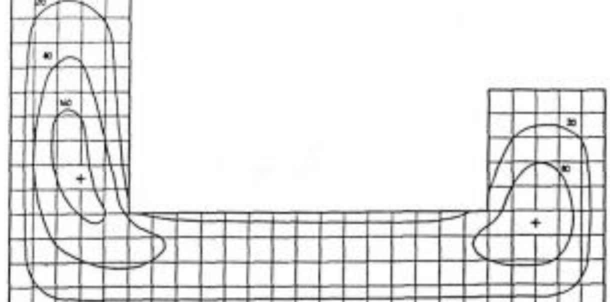
### *4. FLOW DIAGRAM*

*Based on the presented algorithm a computer program was written in ASCII FORTRAN and solved on SPERRY 1100 computer. A detailed flow diagram is seen on **Fig. 2**. The main feature of the program is its use of two temperature matrixes namely T and T*. First matrix contains temperatures at the start and end of time step. The other contains temperature at the end of first $\Delta t/2$. Initial values are assigned to program variables and constants. Program module TYP provides for initial values of temperatures of particular net points as well as for standardization of all points in mold, casting, core and theirs boundary interfaces. Module ISPIS1 prints out initial temperature distribution. The system of tridiagonal equations is then solved firstly row by row (module RED) and then column by column (module STUP). Results are periodically printed over the whole geometry of casting, mold and core (module ISPIS1) or over the casting geometry only (module ISPIS2) untill the prescribed time $t_{max}$.*

### *5. DISCUSSION*

*Simulation of the solidification of 0.25% C steel valve housing casted in sand mold is carried out by space step $\Delta z = \Delta r = 1$ cm and time step $\Delta t = 10$ s till $t_{max} = 200$ s. Casting temperature was 1580°C whereas the initial temperature of mold and core was 25°C. On the basis of successive temperatures print out for particular net points, solidification time 136 s for the right and 181 s for the left heat centre is obtained. The later value is also solidification time for entire casting. By isosolidus shift as seen in **Fig. 3** it can be concluded that potential defect sites are obviously the points of final solidification of heat centres i.e. in the vicinity of inner corner of the casting. From fig. 3 it can be seen that cooling rate of the core is higher than that of the mold since isosolidus curves are shifted outward.*

*The accuracy of the simulation is limited depending on the assumptions utilized in mathematical model, method of numerical analysis and the utilized values of thermophysical material properties. Several assumptions have been used in the elaboration of the mathematical model. The most important are: the heat transfer rate is complete, the casting temperature is equal to initial temperature of metal in the mold and the mold/casting interfacial thermal contact is perfect. The first assumptions restrains the analysis to the mold-casting-*




**Slika 3**
Napredovanje izosolidusa (1449°C) u odljevku za vremena 20, 80 i 140 s.
***Fig. 3***
*Progress of isosolidus (1449°C) after 20, 80 and 140 s.*

la, primjenjenoj metodi numeričke analize i korištenim vrijednostima toplofizičkih svojstava materijala. Pri postavljanju matematičkog modela krenulo se od više pretpostavki od kojih su najvažnije pretpostavka o potpunom provođenju topline, pretpostavka da je temperatura lijevanja jednaka početnoj temperaturi metala u kalupu i pretpostavka o savršenom toplinskom kontaktu na graničnoj plohi kalupa i odljevka. Prva pretpostavka ograničuje razmatranje skrućivanja na sistem kalup-odljevak-jezgra u kojem se toplina prenosi samo provođenjem, što znači da se ne razmatraju parcijalni procesi prijenosa topline vezani uz vlagu u kalupu i jezgri. Druga pretpostavka predstavlja pojednostavljenje uvedeno da se izbjegne kompleksno razmatranje protjecanja metala kroz uljevni sistem i kalupnu šupljinu povezano s prijelazom topline. Pretpostavka o savršenom toplinskom kontaktu na graničnoj plohi odljevka i kalupa prihvatljiva je iz razloga što se na graničnoj plohi tek djelomično javljaju plinski zazori, pa se pri matematičkoj formulaciji uzima da vrijedi granični uvjet četvrte vrste. Parcijalna diferencijalna jednadžba provođenja topline riješena je numeričkom metodom konačne razlike - implicitnom metodom promjenljivog smjera koja je odabrana iz razloga što ima veliku točnost pri aproksimaciji i prostora i vremena. Metoda je drugog reda s obzirom na diskretizaciju prostora i vremena. Nedovoljno poznavanje toplofizičkih svojstava materijala posebno pri visokim temperaturama značajno utječe na simulaciju skrućivanja. To se posebno odnosi na toplinska svojstva kalupnog materijala i jezgre, koja je moguće odrediti samo eksperimentalnim putem a pri visokim temperaturama pokazuje širok dijapazon rasipanja.

## 6. ZAKLJUČAK

U radu je provedena numerička simulacija skrućivanja kućišta ventila od niskougljičnog čeličnog lijeva na formuliranom matematičkom modelu. Modelni sistem je kompleksan jer se sastoji od triju materijala: kalupa, jezgre i odljevka relativno složene geometrije. Matematički model skrućivanja odljevka postavljen je uz pretpostavku da u sistemu postoji samo provođenje topline, što predstavlja fizikalno realnu pretpostavku. Diferencijalna jednadžba provođenja topline koja odgovara geometrijskom uzoru kućišta ventila odgovarajuće je modificirana i riješena numerički implicitnom metodom promjenljivog smjera s time da je uzeta u obzir temperaturna ovisnost toplofizičkih svojstava pojedinih materijala. Na temelju dobivenog algoritma napisan je program u programskom jeziku ASCII FORTRAN za računalo SPERRY 1100. Na temelju simulacije konstatirano je vrijeme skrućivanja od 181 s, a na temelju pomicanja izosolidusa moguće je odrediti tok skurćivanja te mjesta moguće pojave defekta u odljevku.

### Dodatak 1

Popis oznaka korištenih u radu

a — temperaturna vodljivost materijala
$a_i$, $b_i$, $c_i$, $d_i$ — koeficijenti uz nepoznanice u tridijagonalnom sistemu algebarskih jednadžbi
$c_p$ — specifična toplina pri konstantnom tlaku
k — toplinska vodljivost materijala
n — normala
r — prostorna koordinata
t — vrijeme
T — temperatura
$v_i$ — nepoznanica u sistemu simultanih algebarskih jednadžbi
z — prostorna koordinata

*core system with heat conduction only, i.e. partial heat flows associated with mold and core moisture are not considered. The second assumptions is simplification introduced to avoid complex consideration of metal flow through gate system and mold cavity and matching heat transfer. The assumption of perfect thermal contact on the interface is acceptable since only partial appearance of gaseous clearance therefore in mathematical formulation the boundary condition of fourth kind is usually taken as valid. Partial differential equation for heat flow is solved by numerical method of finite difference - the implicit method of variable direction which was chosen due to its high accuracy at approximation of both time and space. The method is of the second order in respect to discretion of time and space. Insufficient knowledge of thermophysical properties of material specially at high temperatures has a strong influence on simulation of the solidification. It holds specially in respect to thermal properties of mold and core material which can be determined only by experiment. Moreover values for thermal properties at higher temperatures show considerable dissipation.*

## 6. CONCLUSIONS

*Numerical simulation of solidification of low carbon steel casting (valve housing) has been carried out on the basis of a suitable mathematical model. The complex model system is composed of three materials: mold, core and casting of comparatively complicated geometry. Mathematical model of solidification has been elaborated assuming thermal conduction as only heat flow in the system which is considered as a physically real assumption. Differential equation for heat flow suited to the geometry of valve housing has been modified and numerically solved by the use of implicit method of variable direction. Temperature dependence of thermophysical material properties has been taken into account. Based on the obtained algorithm a computer program written in ASCII FORTRAN for SPERRY 1100 computer was used for simulation of the solidification. It has been determined that complete solidification takes 181 seconds. The progress of solidification as well as hot spots i.e., sites of potential shrinkage cavities can be determined by shift of isosolidus.*

### *Appendix 1*

*Abbreviations used:*

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

*Indices*

*i - space coordinate z, value for boundary mold/metal surface*
*j - space coordinate r, core*
*k - mold*
*L - casting*
*m - metal*
*s - room, interfacial*

Indeksi

i — prostorna koordinata z, vrijednost na graničnoj plohi kalup-metal
j — prostorna koordinata r, jezgra
k — kalup
L — lijevanje
m — metal
s — sobno, površinski

**Dodatak 2**

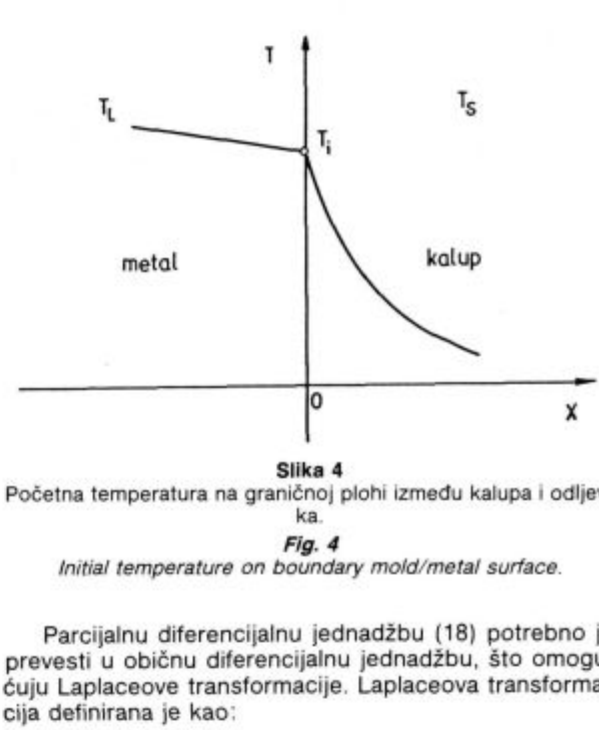
Pri izvođenju jednadžbe za početnu temperaturnu raspodjelu na dodirnoj plohi kalupa i metala potrebno je riješiti parcijalnu diferencijalnu jednadžbu provođenja topline s odgovarjajućim početnim i graničnim uvjetima

$$\frac{\delta T}{\delta t} = a\frac{\delta^2 T}{\delta x^2} \tag{18}$$

$$T(x, O) = T_s \qquad T(O, x) = T_1 \qquad |T(x, t)| < M \tag{19}$$

gdje je M - pozitivna realna konstanta.

Jednadžbu provođenja topline potrebno je riješiti za slučaj kontakta dvaju polubeskonačnih medija, kao što je prikazano na **slici 4**.




**Slika 4**
Početna temperatura na graničnoj plohi između kalupa i odljevka.

***Fig. 4***
*Initial temperature on boundary mold/metal surface.*

Parcijalnu diferencijalnu jednadžbu (18) potrebno je prevesti u običnu diferencijalnu jednadžbu, što omogućuju Laplaceove transformacije. Laplaceova transformacija definirana je kao:

$$\mathcal{L}\{T(x, t)\} = \theta(x, s) = \int_0^\infty e^{-st}\, T(x, t)\, dt \tag{20}$$

Parcijalna diferencijalna jednadžba (18) u Laplaceovom području ima oblik:

$$\frac{d^2\theta}{dx^2} - \frac{1}{a}s\theta = -\frac{1}{a}T_s \tag{21}$$

Riješenje jednadžbe (21) ima oblik:

$$\theta(x\ s) = c_1(s)e^{x\sqrt{s/a}} + c_2(s)\ e^{-x\sqrt{s/a}} + \frac{T_s}{s} \tag{22}$$

***Appendix 2***

*The following partial differential equation of heat flow with appropriate initial and boundary conditions must be solved in order to derive equation for temperature distribution on mold/metal interface.*

$$\frac{\delta T}{\delta t} = a\frac{\delta^2 T}{\delta x^2} \tag{18}$$

$$T(x, O) = T_s \qquad T(O, x) = T_1 \qquad |T(x, t)| < M \tag{19}$$

*where N is a positive real constant.*

*Equation of heat flow should be solved for case of the contact of two semi-infinite media as can be seen in* ***fig. 4****.*

*Partial differential equation (18) must be transformed into common differential equation by Laplace transformation defined as:*

$$\mathcal{L}\{T(x, t)\} = \theta(x, s) = \int_0^\infty e^{-st}\, T(x, t)\, dt \tag{20}$$

*The equation (18) in Laplace region has the form:*

$$\frac{d^2\theta}{dx^2} - \frac{1}{a}s\theta = -\frac{1}{a}T_s \tag{21}$$

*The solution of (21) has the form:*

$$\theta(x\ s) = c_1(s)e^{x\sqrt{s/a}} + c_2(s)\ e^{-x\sqrt{s/a}} + \frac{T_s}{s} \tag{22}$$

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

$$\theta(x,s) = c_2\, e^{-x\sqrt{s/a}} + \frac{T_s}{s} \tag{23}$$

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

$$\theta(O,s) = c_2 + \frac{T_s}{s} = \frac{T_1}{s} \text{ dobije se } c_2 = \frac{1}{s}(T_i - T_s).$$

*Final result in Laplace region is:*

$$\theta(x,s) = \frac{T_i - T_s}{s}\, e^{-x\sqrt{s/a}} + \frac{T_s}{s} \tag{24}$$

*By going out of Laplace region into real space we have:*

$$T(x,t) = (T_i - T_s)\ \mathrm{erfc}\left(\frac{x}{2\sqrt{at}}\right) + T \tag{25}$$

$$\text{odnosno } \frac{T - T_i}{T_s - T_i} = \mathrm{erf}\left(\frac{x}{2\sqrt{at}}\right) \tag{25'}$$

*where the error function is defined as:*

$$\mathrm{erf}\,(t) = \frac{2}{\sqrt{\pi}}\int_0^t e^{-u^2} du \tag{26}$$

*Temperature gradient along x - axis is:*

$$\frac{\delta T}{\delta x} = \frac{T_s - T_i}{\sqrt{\pi a t}} e^{-x^2/4at} \tag{27}$$

$$\text{odnosno } \left(\frac{\delta T}{\delta x}\right) x = o = \frac{T_s - T_i}{\sqrt{\pi a t}} \tag{28}$$

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

Zbog ograničenosti temperature, odnosno $|T(x,t)| < M$ slijedi $c_1 = 0$ za $x \to \infty$, odnosno

$$\theta(x,s) = c_2\, e^{-x\sqrt{s/a}} + \frac{T_s}{s} \tag{23}$$

Korištenjem graničnog uvjeta $T(0,t) = T_i$, odnosno

$$\theta(O,s) = c_2 + \frac{T_s}{s} = \frac{T_1}{s} \text{ dobije se } c_2 = \frac{1}{s}(T_i - T_s).$$

Konačni rezultat u Laplaceovom području je

$$\theta(x,s) = \frac{T_i - T_s}{s} e^{-x\sqrt{s/a}} + \frac{T_s}{s} \tag{24}$$

Prijelazom iz Laplaceovog područja u realno područje dobije se

$$T(x,t) = (T_i - T_s) \text{ erfc } \left(\frac{x}{2\sqrt{at}}\right) + T \tag{25}$$

$$\text{odnosno } \frac{T - T_i}{T_s - T_i} = \text{ erf } \left(\frac{x}{2\sqrt{at}}\right) \tag{25'}$$

pri čemu je funkcija pogreške definirana kao

$$\text{erf }(t) = \frac{2}{\sqrt{\pi}} \int_0^t e^{-u^2} du \tag{26}$$

Temperaturni gradijent u smjeru osi x je:

$$\frac{\delta T}{\delta x} = \frac{T_s - T_i}{\sqrt{\pi a t}} e^{-x^2/4at} \tag{27}$$

$$\text{odnosno } \left(\frac{\delta T}{\delta x}\right) x = o = \frac{T_s - T_i}{\sqrt{\pi a t}} \tag{28}$$

Na graničnoj plohi u kontaktu su dva polubeskonačna medija (kalup i metal) pri čemu vrijedi granični uvjet četvrte vrste:

$$-k_k \left(\frac{\delta T_k}{\delta x}\right) x = 0 = -k_m \left(\frac{\delta T_m}{\delta x}\right) x = 0 \tag{29}$$

Uvrštavanjem odgovarajućih gradijenata temperature dobije se

$$k_k \frac{T_i - T_s}{\sqrt{\pi a_k t}} = k_m \frac{T_L - T_i}{\sqrt{\pi a_m t}} \tag{30}$$

Sređivanjem jednadžbe (30) dobije se početna temperaturna raspodjela na graničnoj plohi između kalupa i odljevka

$$T_i = T_s + \frac{T_L + T_s}{1 + \frac{k_k}{k_m}\sqrt{\frac{a_m}{a_k}}} \tag{31}$$

**Dodatak 3**

Toplofizička svojstva materijala

a) Niskougljični čelični lijev (oko 0,25% C)

Toplinska vodljivost, W/mK

| | |
|---|---|
| $T \geq 1499^0 C$ | $k = 25{,}96$ |
| $1499^0 C > T \geq 1449^0 C$ | $k = 207{,}54 - 0{,}12114\, T$ |
| $1499^0 C > T \geq 893^0 C$ | $k = 26{,}6 + 0{,}00374\, T$ |
| $893^0 C > T$ | $k = 50{,}31 - 0{,}0225\, T$ |

Specifična toplina, J/kgK

$$-k_k \left(\frac{\delta T_k}{\delta x}\right) x = 0 = -k_m \left(\frac{\delta T_m}{\delta x}\right) x = 0 \tag{29}$$

*By including proper temperature gradients:*

$$k_k \frac{T_i - T_s}{\sqrt{\pi a_k t}} = k_m \frac{T_L - T_i}{\sqrt{\pi a_m t}} \tag{30}$$

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

$$T_i = T_s + \frac{T_L + T_s}{1 + \frac{k_k}{k_m}\sqrt{\frac{a_m}{a_k}}} \tag{31}$$

***Appendix 3***

*Thermo-physical properties of the materials*

*a) Low carbon (0.25% C) casted steel*

*Thermal conductivity, W/mK*

| | |
|---|---|
| $T \geq 1499^0 C$ | $k = 25{,}96$ |
| $1499^0 C > T \geq 1449^0 C$ | $k = 207{,}54 - 0{,}12114\, T$ |
| $1499^0 C > T \geq 893^0 C$ | $k = 26{,}6 + 0{,}00374\, T$ |
| $893^0 C > T$ | $k = 50{,}31 - 0{,}0225\, T$ |

*Specific heat, J/kgK*

| | |
|---|---|
| $T \geq 1499^0 C$ | $c_p = 879{,}2$ |
| $1499^0 C > T \geq 1474^0 C$ | $c_p = 652273{,}5 - 434{,}585\, T$ |
| $1474^0 C > T \geq 1449^0 C$ | $c_p = 436{,}258\, T - 631251{,}9$ |
| $1449^0 C > T \geq 982^0 C$ | $c_p = 421{,}36 + 0{,}28712\, T$ |
| $982^0 C > T \geq 704^0 C$ | $c_p = 1502{,}8 - 0{,}81391\, T$ |
| $704^0 C > T \geq 427^0 C$ | $c_p = 143{,}76 + 1{,}11535\, T$ |
| $427^0 C > T$ | $c_p = 458{,}86 + 0{,}37681\, T$ |

*b) Core*

*Thermal conductivity, W/mK*

$k = 3.246 \times 10^{-6}\, T^2 - 3.894 \times 10^{-3} T + 3.052$

*Temperature diffusivity, $m^2/s$*

$a = 1.689 \times 10^{-12}\, T^2 - 2.174 \times 10^{-9} T + 1.785 \times 10^{-6}$

*c) Mold*

*Thermal conductivity, W/mK*

$k = 3.937 \times 10^{-6} T^2 - 3.57 \times 10^{-3} T + 3.421$

*Temperature diffusivity, $m^2/s$*

$a = 1.957 \times 10^{-12} T^2 - 1.8 \times 10^{-9} T + 1.913 \times 10^{-6}$

***Appendix 4***

*Constants which appear in tridiagonal coefficients*

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

$$p_2 = \frac{a\, \Delta t}{4 r_i \Delta r}$$

$$p_3 = p_1 - p_2$$

$$p_4 = p_i + p_2$$

$$p_5 = \frac{\Delta t\, (k_A + k_B)}{2\, c\, (\Delta r)^2}$$

$$p_6 = \frac{\Delta t\, (k_A + k_B)}{4\, c\, r_i \Delta r}$$

$$c = \frac{k_A}{a_A} + \frac{k_B}{a_B}$$

| | |
|---|---|
| $T \geq 1499^0 C$ | $c_p = 879{,}2$ |
| $1499^0 C > T \geq 1474^0 C$ | $c_p = 652273{,}5 - 434{,}585\ T$ |
| $1474^0 C > T \geq 1449^0 C$ | $c_p = 436{,}258\ T - 631251{,}9$ |
| $1449^0 C > T \geq 982^0 C$ | $c_p = 421{,}36 + 0{,}28712\ T$ |
| $982^0 C > T \geq 704^0 C$ | $c_p = 1502{,}8 - 0{,}81391\ T$ |
| $704^0 C > T \geq 427^0 C$ | $c_p = 143{,}76 + 1{,}11535\ T$ |
| $427^0 C > T$ | $c_p = 458{,}86 + 0{,}37681\ T$ |

b) Jezgra

Toplinska vodljivost, W/mK
$k = 3{,}246 \cdot 10^{-6}\, T^2 - 3{,}894 \cdot 10^{-3} T + 3{,}052$
Temperaturna vodljivost, $m^2/s$
$a = 1{,}689 \cdot 10^{-12} T^2 - 2{,}174 \cdot 10^{-9}\, T + 1{,}785 \cdot 10^{-6}$

c) Kalup

Toplinska vodljivost, W/mK
$k = 3{,}937 \cdot 10^{-6}\, T^2 - 3{,}57 \cdot 10^{-3}\, T + 3{,}421$
Temperaturna vodljivost, $m^2/s$
$a = 1{,}957 \cdot 10^{-12}\, T^2 - 1{,}8 \cdot 10^{-9}\, T + 1{,}913 \cdot 10^{-6}$

**Dodatak 4**

Konstante koje se javljaju u tridijagonalnim koeficijentima

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

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

$$p_3 = p_1 - p_2$$

$$p_4 = p_i + p_2$$

$$p_5 = \frac{\Delta t\ (k_A + k_B)}{2\ c\ (\Delta r)^2}$$

$$p_6 = \frac{\Delta t\ (k_A + k_B)}{4\ c\ r_j \Delta r}$$

$$c = \frac{k_A}{a_A} + \frac{k_B}{a_B}$$

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

$$q_2 = \frac{K_A \Delta t}{c\ (\Delta z)^2}$$

$$q_3 = \frac{k_A \Delta t}{c\ (\Delta z)^2}$$

$$q_4 = \frac{\Delta t\ (k_A + k_B)}{2\ c\ (\Delta z)^2}$$

$$q_5 = \frac{K_A sa40D'}{c\ (\Delta r)^2}$$

$$q_6 = \frac{k_B \Delta t}{c\ (\Delta r)^2}$$

Tridijagonalni koeficienti
1. Točka (i,j) u kalupu, metalu odnosno jezgri
— prvi $\Delta t/2$:

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

$$q_2 = \frac{K_A \Delta t}{c\ (\Delta z)^2}$$

$$q_3 = \frac{k_A \Delta t}{c\ (\Delta z)^2}$$

$$q_4 = \frac{\Delta t\ (k_A + k_B)}{2\ c\ (\Delta z)^2}$$

$$q_5 = \frac{K_A sa40D'}{c\ (\Delta r)^2}$$

$$q_6 = \frac{k_B \Delta t}{c\ (\Delta r)^2}$$

*Tridiagonal coefficients*
*1. Point (i,j) in the mold, metal or core; first* $\Delta t/2$:

$$a_i = c_i = -q_1$$
$$b_i = 1 + 2\, q_1$$
$$d_i = p_3\, T^n_{i,j-1} + (1 - 2p_1)\, T^n_{i,j} + p_4 T^n_{i,j+1} \qquad (32)$$

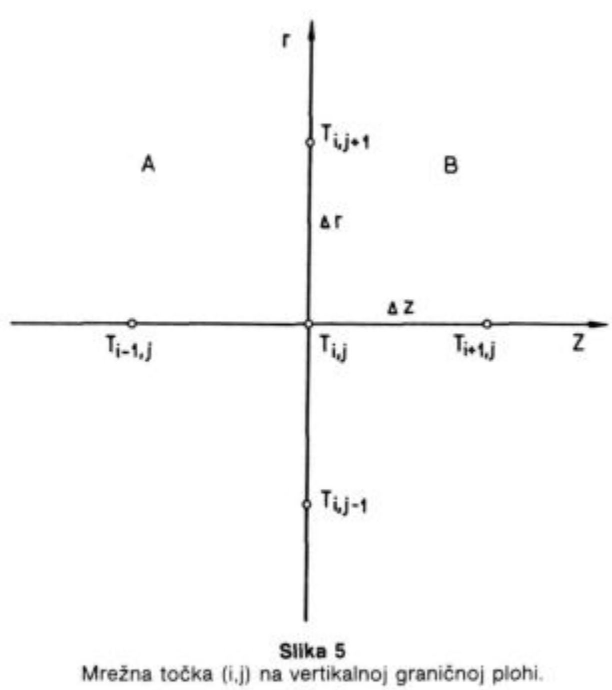
— *second* $\Delta t/2$:

$$a_i = -p_3$$
$$b_i = 1 + 2\, p_1$$
$$c_i = -p_4$$
$$d_i = q_1\, T^{n+1/2}_{i-1,j} + (1 - 2q_1)\, T^{n+1/2}_{i,j} + q_1\, T^{n+1/2}_{i+1,j} \qquad (33)$$

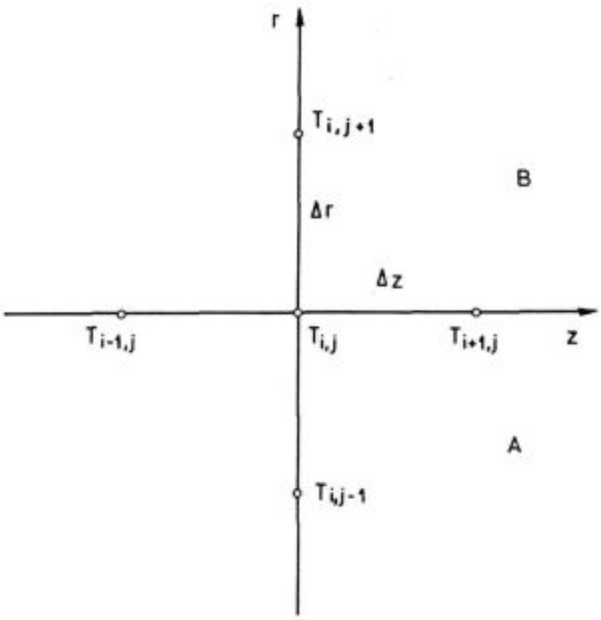
*2. Point (i,j) on the boundary surface parallel to r axis separating the material A (left) and B (right).*

— *first* $\Delta t/2$:

$$a_i = -q_2$$
$$b_i = 1 + q_2 + q_3$$
$$c_i = q_3$$
$$d_i = (p_5 - p_6)\, T^n_{i,j-1} + (1 - 2p_5)\, T^n_{i,j} + (p_5 + p_6)\, T^n_{i,j+1} \qquad (34)$$




**Slika 5**
Mrežna točka (i,j) na vertikalnoj graničnoj plohi.
***Fig. 5***
*Net point (i,j) on vertical boundary surface.*




**Slika 6**
Mrežna točka (i,j) na horizontalnoj graničnoj plohi.
***Fig. 6***
*Net point (i,j) on horizontal boundary surface.*

$$a_i = c_i = -q_1$$
$$b_i = 1 + 2\,q_1$$
$$d_i = p_3\,T^n_{i,j-1} + (1-2p_1)\,T^n_{i,j} + p_4 T^n_{i,j+1} \qquad (32)$$

— drugi $\Delta t/2$:

$$a_j = -p_3$$
$$b_j = 1 + 2\,p_1$$
$$c_j = -p_4$$
$$d_j = q_1\,T^{n+1/2}_{i-1,j} + (1-2q_1)\,T^{n+1/2}_{i,j} + q_1\,T^{n+1/2}_{i+1,j} \qquad (33)$$

2. Točka (i,j) na graničnoj plohi paralelno r osi koja odvaja materijal A (lijevo) i B (desno)
— prvi $\Delta t/2$:

$$a_i = -q_2$$
$$b_i = 1 + q_2 + q_3$$
$$c_i = q_3$$
$$d_i = (p_5 - p_6)\,T^n_{i,j-1} + (1-2p_5)\,T^n_{i,j} + (p_5 + p_6)\,T^n_{i,j+1} \qquad (34)$$

— drugi $\Delta t/2$:
$$a_j = -(p_5 - p_6)$$
$$b_j = 1 + 2\,p_5$$
$$c_j = -(p_5 + p_6)$$
$$d_j = q_2\,T^{n+1/2}_{i-1,j} + (1-q_2-q_3)\,T^{n+1/2}_{i,j} + q_3\,T^{n+1/2}_{i+1,j} \qquad (35)$$

3. Točka (i, j) na graničnoj plohi paralelno z osi koja dijeli materijal A (dolje) i B (gore)

— prvi $\Delta t/2$:
$$a_i = c_i = -q_4$$
$$b_i = 1 + 2q_4$$
$$d_i = (q_5 - q_6)\,T^n_{i,j-1} + (1-2p_5)\,T^n_{i,j} + (q_6 + p_6)\,T^n_{i,j+1} \qquad (36)$$

— drugi $\Delta t/2$:
$$a_j = p_6 - q_5$$
$$b_j = 1 + 2p_5$$
$$c_j = -(q_6 + p_6)$$
$$d_j = q_4\,T^{n+1/2}_{i-1,j} + (1\text{-}2q_4)T^{n+1/2}_{i,j} + q_4\,T^{n+1/2}_{i+1,j} \qquad (37)$$

— *second* $\Delta t/2$:
$$a_j = -(p_5 - p_6)$$
$$b_j = 1 + 2\,p_5$$
$$c_j = -(p_5 + p_6)$$
$$d_j = q_2\,T^{n+1/2}_{i-1,j} + (1-q_2-q_3)\,T^{n+1/2}_{i,j} + q_3\,T^{n+1/2}_{i+1,j} \qquad (35)$$

*3. Point (i,j) on the boundary surface parallel to z axis separating the material A (down) and B (up).*
— *first* $\Delta t/2$:
$$a_i = c_i = -q_4$$
$$b_i = 1 + 2q_4$$
$$d_i = (q_5 - q_6)\,T^n_{i,j-1} + (1-2p_5)\,T^n_{i,j} + (q_6 + p_6)\,T^n_{i,j+1} \qquad (36)$$

— *second* $\Delta t/2$:
$$a_j = p_6 - q_5$$
$$b_j = 1 + 2p_5$$
$$c_j = -(q_6 + p_6)$$
$$d_j = q_4\,T^{n+1/2}_{i-1,j} + (1\text{-}2q_4)T^{n+1/2}_{i,j} + q_4\,T^{n+1/2}_{i+1,j} \qquad (37)$$

*4. Point (i,1) out of boundary surface; first* $\Delta t/2$:

$$a_i = c_i = -q_1$$
$$b_i = 1 + 2q_1$$
$$d_i = (1-4p_1)\,T^n_{i,1} + 4p_1\,T^n_{i,2} \qquad (38)$$

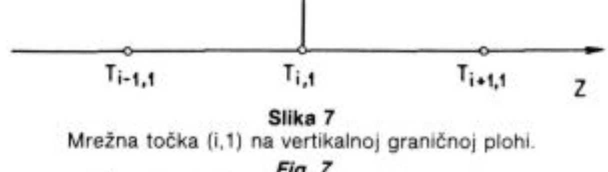
— *second* $\Delta t/2$:

$$b_j = 1 + 4p_1$$
$$c_j = 4p_1$$
$$d_j = q_1\,T^{n+1/2}_{i-1,1} + (1-2q_1)\,T^{n+1/2}_{i,1} + q_1\,T^{n+1/2}_{i+1,1} \qquad (39)$$

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

— *first* $\Delta t/2$ :
$$a_i = -q_2$$
$$b_i = 2q_4 + 1$$
$$c_i = -q_3$$
$$d_i = (1-4p_5)\,T^n_{i,1} + 4p_5\,T^n_{i,2} \qquad (40)$$

— *second* $\Delta t/2$:
$$b_j = 4p_5 + 1$$
$$c_j = -4p_5$$
$$d_j = q_2\,T^{n+1/2}_{i-1,1} + (1-2q_4)\,T^{n+1/2}_{i,1} + q_3\,T^{n+1/2}_{i+1,1} \qquad (41)$$




**Slika 7**
Mrežna točka (i,1) na vertikalnoj graničnoj plohi.
***Fig. 7***
*Net point (i,1) on vertical boundary surface.*

**4**. Točka (i, 1) koja nije na granici

— prvi $\Delta t/2$:

$$a_i = c_i = -q_1$$
$$b_i = 1 + 2q_1$$
$$d_i = (1-4p_1)\, T^n_{i,1} + 4p_1\, T^n_{i,2} \qquad (38)$$

— drugi $\Delta t/2$:

$$b_j = 1 + 4p_1$$
$$c_j = 4p_1$$
$$d_j = q_1\, T^{n+1/2}_{i-1,1} + (1-2q_1)\, T^{n+1/2}_{i,1} + q_1\, T^{n+1/2}_{i+1,1} \qquad (39)$$

5. Točka (i, 1) na graničnoj plohi koja dijeli material A (lijevo) i B (desno)

— prvi $\Delta t/2$:

$$a_i = -q_2$$
$$b_i = 2q_4 + 1$$
$$c_i = -q_3$$
$$d_i = (1-4p_5)\, T^n_{i,1} + 4p_5\, T^n_{i,2} \qquad (40)$$

— drugi $\Delta t/2$:

$$b_j = 4p_5 + 1$$
$$c_j = -4p_5$$
$$d_j = q_2\, T^{n+1/2}_{i-1,1} + (1-2q_4)\, T^{n+1/2}_{i,1} + q_3\, T^{n+1/2}_{i+1,1} \qquad (41)$$

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