METRO
MEtallurgical TRaining On-line

Computer modeling of phase transformation of cast alloys in solid state especially taking into consideration ADI castings

Lecture III: Finite Difference Method for heat and mass transfer

Wojciech Kapturkiewicz

AGH

Education and Culture

Finite Difference Method

Introduction

The processes of heat conduction and mass transfer in ADI technology are described by Parabolic Equations, which can be solved numerically by application of the Finite Difference Method (FDM) or Finite Element Method (FEM).

Heat Conduction Equation (Fourier's Law) has the form identical as Mass Transfer Equation (Fick's Law). Therefore, to examine both these processes it is enough to examine only one of them, e.g. the process of heat conduction. When the mass transfer is examined, the term ***heat diffusivity "a"*** will be replaced with the term ***mass diffusivity "D",*** expressed in the same units *(m^2/s)*. Some differences may occur, however, in boundary conditions or the problem of *moving phase boundary* (which is presented in Lecture II, eqs. 3 - 10).

There the simple version of the FDM is presented.

Finite Difference Method

(The simple version)

A differential equation with partial derivatives is solved by solving a system of algebraic equations, the number of which equals the number of nodes in a discretisation network.

The method of the variables discretisation will be discussed on an example of the differential equation of heat conduction in a one-dimensional plane solid body without any internal heat sources and with the value of *thermal diffusivity ”a”* kept constant:

$$\frac{\partial T}{\partial \tau} = a \frac{\partial^2 T}{\partial x^2} \qquad (1)$$

where: T – temperature,
τ - time,
x – co-ordinate.

Finite Difference Method

The left side of the equation (1) can be replaced with the first member of Taylor's sequence:

$$\left(\frac{\partial T}{\partial \tau}\right)_i^k = \frac{T_i^{k+1} - T_i^k}{\Delta \tau} - \frac{\Delta \tau}{2!}\left(\frac{\partial^2 T}{\partial \tau^2}\right)_i^k + \ldots \approx \frac{T_i^{k+1} - T_i^k}{\Delta \tau}$$

or, depending on the mode of expansion, the derivative is replaced with differential quotient

forward (Fig.1): $$\left(\frac{\partial T}{\partial \tau}\right)_i^k = \frac{T_i^{k+1} - T_i^k}{\Delta \tau} \qquad (2)$$

backward: $$\left(\frac{\partial T}{\partial \tau}\right)_i^k = \frac{T_i^k - T_i^{k-1}}{\Delta \tau}$$

or central: $$\left(\frac{\partial T}{\partial \tau}\right)_i^k \approx \frac{T_i^{k+1} - T_i^{k-1}}{2\,\Delta \tau}$$

where $\Delta\tau$ – time step

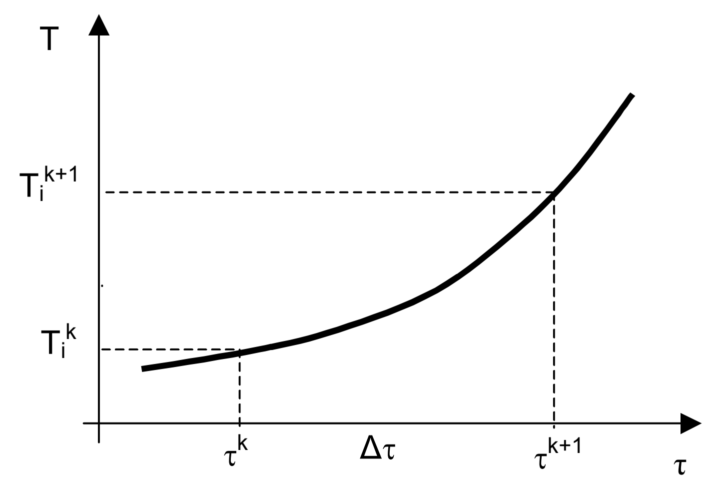


Fig.1. Temperature – time function

Finite Difference Method

The most frequently applied, and at the same time the easiest for computation, is approximation with forward differential quotient of the left side of the differential equation.

The right side of the differential equation of heat conduction, i.e. the temperature derivative with respect to space, is computed with central differential quotient of the second order (Fig. 2):

$$\left(\frac{\partial^2 T}{\partial x^2}\right)_i^k \approx \frac{\dfrac{T_{i-1}^k - T_i^k}{\Delta x} - \dfrac{T_i^k - T_{i+1}^k}{\Delta x}}{\Delta x} = \frac{T_{i-1}^k - 2T_i^k + T_{i+1}^k}{\Delta x^2} \qquad (3)$$

where Δx — distance step

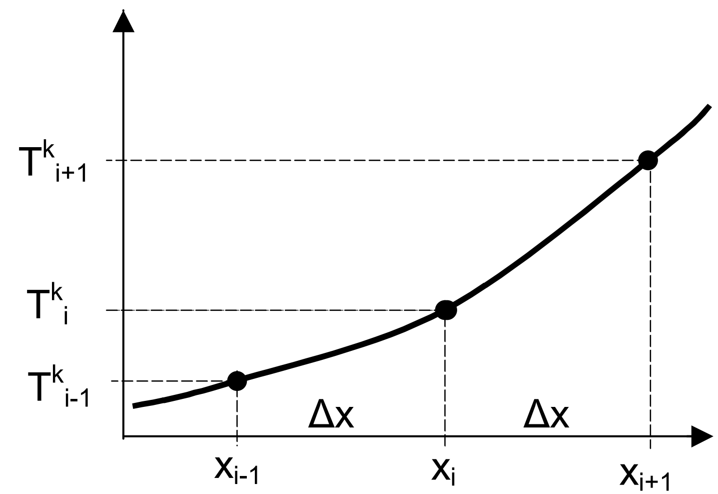


Fig.2. Temperature – distance relation

Finite Difference Method

By combining (1), (2) and (3) we obtain:

$$\frac{T_i^{k+1} - T_i^k}{\Delta \tau} = a \frac{T_{i-1}^k - 2T_i^k + T_{i+1}^k}{\Delta x^2}$$

After transformation with respect to unknown, we obtain a differential equation with explicit system and bottom-up approximation with respect to accurate solution:

$$T_i^{k+1} = T_i^k (1 - 2F) + (T_{i-1}^k + T_{i+1}^k) F \qquad (4)$$

where: $F = \frac{a \Delta \tau}{\Delta x^2}$ (Fourier's difference criterion)

For mass diffusion the adequate criterion is: $F_D = \frac{D \Delta \tau}{\Delta x^2}$

where D – mass diffusivity, m^2/s

Finite Difference Method

The equation (4) keeps the physical point if the value of F (from the definition - positive) doesn't affect on the direction of temperature T_i^{k+1} change.
It is done if:

$$(1-2F)\geq 0$$

and then the stability condition is:

$$F \leq 1/2 \qquad (5)$$

Finite Difference Method

Crank –Nicolson method

In Crank-Nicolson's method, as an approximate value of temperature with respect to time, the differential symmetrical quotient at the time instant k+0,5 has been used; it gives approximate values oscillating around the true value of accurate solution.

To make approximation of the temperature derivative, a forward differential quotient is used:

$$\left(\frac{\partial T}{\partial \tau}\right)_i^{k+0,5} \approx \frac{T_i^{k+1} - T_i^{k}}{\Delta \tau}$$

while the second temperature derivative with respect to space coordinate is replaced by an arithmetic mean of the symmetrical differential quotients of the second order at time intervals k+1 and k:

Finite Difference Method

Crank –Nicolson Method

$$\left(\frac{\partial^2 T}{\partial x^2}\right)_i^{k+0,5} \approx \frac{1}{2\,\Delta x}\left(\frac{T_{i+1}^{k+1}-T_i^{k+1}}{\Delta x}-\frac{T_i^{k+1}-T_{i-1}^{k+1}}{\Delta x}+\frac{T_i^{k+1}-T_i^{k}}{\Delta x}-\frac{T_i^{k}-T_{i-1}^{k}}{\Delta x}\right)$$

By substituting the approximations to (1) we obtain:

$$\frac{T_i^{k+1}-T_i^{k}}{\Delta\tau}=\frac{a}{2\left(\Delta x\right)^2}\left(T_{i+1}^{k+1}-2T_i^{k+1}+T_{i+1}^{k}-2T_i^{k}+T_{i-1}^{k}\right)$$

wherefrom, having allowed for a definition of F number, we obtain:

$$T_i^{k+1}=\frac{1-F}{1+F}T_i^{k}+\frac{F}{2(1+F)}\left(T_{i+1}^{k+1}+T_{i-2}^{k+1}+T_{i+1}^{k}+T_{i-1}^{k}\right)$$

Finite Difference Method

Crank –Nicolson Method

Due to high accuracy of the derivative approximation, large time steps can be applied, and for this reason Crank-Nicolson's method is considered to be a differential tool most effective in computation of the non-steady heat conduction (in one-dimensional system).

Finite Difference Method

Balance Method

Equation (4) can be derived by balancing the steady heat (or mass) flux flow. The method is specially suitable when combining the equations for a non-homogeneous network, comprising different space steps and characterised by different thermophysical parameters.

Let us isolate in a one-dimensional space three plane elements of a linear dimension Δx. The centres of these elements at the time level k will have temperatures amounting to T_{i-1}, T_i and T_{i+1}, respectively (Fig.3).

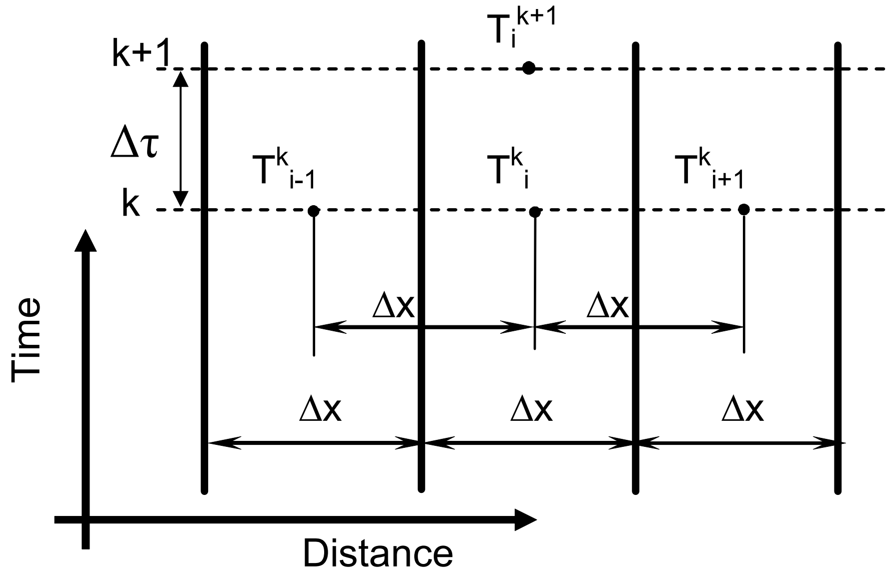


Fig. 3.

Finite Difference Method

Balance Method

Assuming that, at a given time interval $\Delta\tau$, the heat conduction is steady and the thermophysical parameters λ, c and ρ are constant, the heat balance for a middle element of temperature T_i can be written down as:

$$\frac{\lambda}{\Delta x}\left(T_{i-1}^{k}-T_{i}^{k}\right)\Delta\tau+\frac{\lambda}{\Delta x}\left(T_{i+1}^{k}-T_{i}^{k}\right)\Delta\tau=c\rho\Delta x\left(T_{i}^{k+1}-T_{i}^{k}\right) \qquad (6)$$

where λ, c, ρ - heat conductivity, heat capacity and density

The above balance is next transformed to form equation (4):

$$T_{i}^{k+1}=T_{i}^{k}(1-2F)+(T_{i-1}^{k}+T_{i+1}^{k})\,F$$

Finite Difference Method

The dimensionless form of differential equation

One can use in computations any arbitrary temperature scale, and hence equation (4) is written down in the form of:

$$\Theta_i^{k+1} = \Theta_i^k (1-2F) + (\Theta_{i-1}^k + \Theta_{i+1}^k) F$$

where:

$$\Theta_{i-1}^k = \frac{T_{i-1}^k - T_{srf}}{T_0 - T_{srf}} \qquad \Theta_{i+1}^k = \frac{T_{i+1}^k - T_{srf}}{T_0 - T_{srf}}$$

$$\Theta_{i-1}^k = \frac{T_{i-1}^k - T_{amb}}{T_0 - T_{amb}} \qquad \Theta_{i+1}^k = \frac{T_{i+1}^k - T_{amb}}{T_0 - T_{amb}}$$

T_{srf}, T_{amb} – surface and ambient temperature

Finite Difference Method

The differential equation for a system boundary

Boundary condition of the 3rd type

The differential equation for the temperature of an element located near the body surface can be derived by the elementary balance method. The heat balance made for a near-surface element has the form of (Fig. 4):

$$\frac{\lambda}{\Delta x}\left(T_{n-1}^{k}-T_{n}^{k}\right)\Delta\tau+\frac{T_{amb}-T_{n}^{k}}{\dfrac{\Delta x}{2\lambda}+\dfrac{1}{\alpha}}\Delta\tau=c\rho\Delta x\left(T_{n}^{k+1}-T_{n}^{k}\right) \qquad (7)$$

where α - heat transfer coefficient, $\mathrm{W/m^2K}$

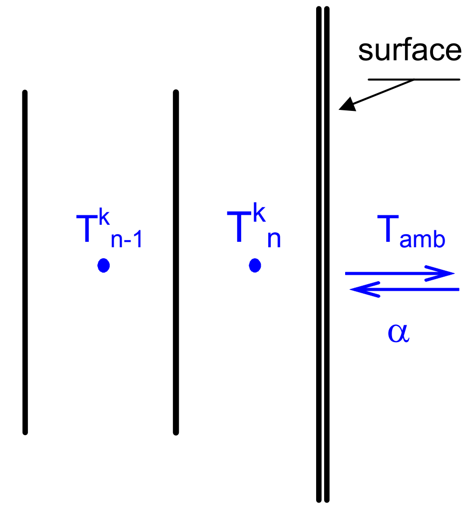


Fig. 4

Finite Difference Method

Boundary condition of the 3rd type

The term $\left(\frac{\Delta x}{2\lambda}+\frac{1}{\alpha}\right)$ in equation (7) expresses heat resistance between the centre of border element and its environment.

Transforming equation (7) we obtain:

$$T_i^{k+1} = T_i^k(1-F-G) + T_{i-1}^k F + T_{i+1}^k G \qquad (8)$$

but for i = n $T_{i+1}^k = T_{amb}$ $\qquad G = \frac{2FN}{2+N}$ $\qquad N = \frac{\alpha}{\lambda}\Delta x$

The dimensionless parameter *N* has the sense of Biot's criterion referred to the dimension of a differential element Δx, and as such can be called Biot's differential criterion. On the other hand, the quantity *G* can be called differential criterion of the (most typical) boundary condition of the *3rd* type.

Finite Difference Method

Boundary condition of the 3rd type

The condition for stability of computations according to equation (8) is to have:

$$1 - F - G \geq 0$$

that is $$1 - F - \frac{2FN}{2+N} \geq 0$$

From the above inequality it follows that: $$N \geq \frac{2F - 2}{1 - 3F}$$

Having previously assumed that $F<1/3$, the above condition is always satisfied, since for this value of F the right side of the inequality assumes a negative value, while the left side (criterion N) is, on account of its physical sense, positive.

Finite Difference Method

Boundary condition of the 3rd type

Preferably, equation (8) can be written down in a more general form as:

$$T_i^{k+1} = T_i^k (1 - A_i - B_i) + T_{i-1}^k A_i + T_{i+1}^k B_i \tag{9}$$

Parameters A_i and B_i illustrate (for the conventionally adopted system of coordinates) the heat effect exerted on element *"i"* by elements located on its left and right side, respectively.

Equation (9) may be considered a general form of equation (4), where criteria A_i and B_i have assumed values dependent on the location of element "i" within the domain of *1D* network:

Criterion/ Element no	A_i	B_i
$i = 1$	0	F
$i \in (2,\, n-1)$	F	F
$i = n$	F	$\frac{2FN}{2+N}$

Finite Difference Method

Introducing the notion of phase transformation

The heat of solidification, constant solidification temperature

The phase transformation most important in castings is the transformation of metal from liquid to a solid state, combined with release of the latent heat of transformation, i.e. the heat of solidification. How important quantitatively is this transformation can be evaluated dividing the value of the heat of solidification of the examined metal or alloy by the value of its specific heat. Then we shall obtain a number H, expressed in degrees $[K]$, which can be considered “temperature reserve of the heat of solidification”.

For a typical cast iron:

solidification heat L = 270 J/g

specific heat c = (0.753 + 0.837)/2 = 0.795 J/g K (mean specific heat for liquid and solid state

is obtained: H = L/c = 270/0.795 ≈ 340 K.

Finite Difference Method

Heat of Solidification

Dividing the value of H by the value of the transformation temperature we get the significance level of the heat of transformation. The significance of the heat of transformation S_L, assuming the solidification temperature of cast iron is T_{kr}, is:

$$S_L = H/T_{kr} \approx 0.29$$

It can be assumed further that from the moment when the solidifying but still liquid metal has reached the temperature of transformation, it possesses a "temperature reserve of the heat of solidification", which means that the temperature of a given element will not drop below the solidification point as long as the temperature "reserve" is not completely exhausted, that is, as long as the condition:

$$\sum_k \Delta T_i^k \leq H \qquad (10)$$

is satisfied.

where $\Delta T_i^k = T_{kr} - T_i^{k+1}$ - temperature drop at a given time step below the solidification point.

Finite Difference Method

Heat of Solidification

If condition (10) is satisfied, then the temperature will be maintained at a constant level, that is ($T_i^{k+1} = T_{kr}$). Hence, the time necessary to exhaust the temperature reserve *H* will equal the time of metal solidification within the domain of a given differential element.

Finite Difference Method

Heat of Solidification

Range of Solidification Temperature

The heat of solidification within a temperature range ΔT_{kr} can be introduced through application of the term of an effective specific heat:

$$c_{ef} = c + \frac{L}{\Delta T_{kr}} \tag{11}$$

where $\Delta T_{kr} = T_{lik} - T_{sol}$

T_{lik} and T_{sol} - temperature liquidus and solidus for an alloy

When the temperature of a given differential element is within the range of ΔT_{kr}, then F in the differential equations should be replaced with (for $T_{sol} \le T_i^k \le T_{lik}$):

$$F_{ef} = \frac{a_{ef} \Delta \tau}{\Delta x^2} \tag{12}$$

where $a_{ef} = \frac{\lambda}{c_{ef} \rho}$ λ - heat conductivity, ρ - density

Finite Difference Method

Heat of Solidification

Range of Solidification Temperature

When a function of the spectral heat of solidification η_T is available (for example of the type ($\eta_T = A_0 + A_1 T + A_2 T^2$)), we can also use the term of an effective specific heat c_{ef} and F_{ef}, respectively, computing its value for the actual metal temperature (the temperature at a given differential interval), under the assumption that:

$$c_{ef} = c + \eta_T \qquad (13)$$

where $\eta_T = A_0 + A_1 T + A_2 T^2$

A_0, A_1, A_2 – regression coefficients

Finite Difference Method

General form of equation for one-dimensional (1D) system

Let us assume that the differential elements have different dimensions and different thermophysical properties. For a unidirectional heat conduction (Fig. 3) the elementary heat balance can be written down as:

$$\frac{(T_{i-1}^{k} - T_{i}^{k})\Delta\tau}{\frac{\Delta x_{i-1}}{2\lambda_{i-1}} + \frac{\Delta x_{i}}{2\lambda_{i}}} + \frac{(T_{i+1}^{k} - T_{i}^{k})}{\frac{\Delta x_{i}}{2\lambda_{i}} + \frac{\Delta x_{i+1}}{2\lambda_{i+1}}} = c_{i}\rho_{i}\Delta x_{i}(T_{i}^{k+1} - T_{i}^{k})$$

where *"i"* – the index of parameters referred to the *i-th* differential element.

After transformation we obtain equation as (9):

$$T_{i}^{k+1} = T_{i}^{k}(1 - A_{i} - B_{i}) + T_{i-1}^{k}A_{i} + T_{i+1}^{k}B_{i} \qquad (14)$$

Finite Difference Method

General form of equation for one-dimensional (1D) system

where $A_i = \dfrac{2F_i}{1 + \dfrac{\lambda_i \Delta x_{i-1}}{\lambda_{i-1} \Delta x_i}}$ $B_i = \dfrac{2F_i}{1 + \dfrac{\lambda_i \Delta x_{i+1}}{\lambda_{i+1} \Delta x_i}}$ $F_i = \dfrac{a_i \Delta\tau}{\Delta x_i^2}$ $a_i = \dfrac{\lambda_i}{c_i \rho_i}$

The stability condition of solution is to have: $(A_i + B_i) \le 1$

If we assume a uniform differential division, then the constants in equation (14) will have the form of:

$$A_i = \frac{2F_i}{1 + \dfrac{\lambda_i}{\lambda_{i-1}}} \qquad B_i = \frac{2F_i}{1 + \dfrac{\lambda_i}{\lambda_{i+1}}}$$

If, additionally, the differential elements will have the same coefficients of heat conduction (a homogeneous system), then:

$$A_i = B_i = F$$

and equation (14) will assume the form of equation (4): $T_i^{k+1} = T_i^k (1 - 2F) + (T_{i-1}^k + T_{i+1}^k) F$

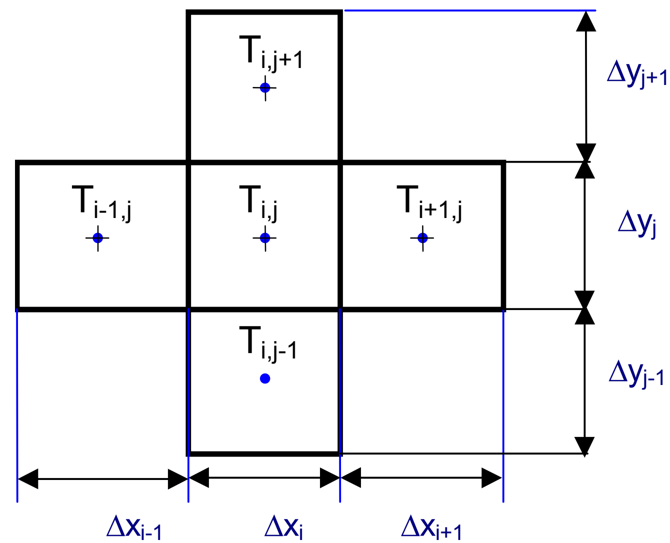
Finite Difference Method

Two-dimensional system (2D)

For a two-dimensional network system, the differential equation can be derived by the elementary balance method (Fig. 5):

$$\frac{(T^k_{i-1,j} - T^k_{i,j})\Delta\tau\Delta y_j}{\dfrac{\Delta x_{i-1}}{2\lambda_{i-1,j}} + \dfrac{\Delta x_i}{2\lambda_{i,j}}} + \frac{(T^k_{i+1,j} - T^k_{i,j})\Delta\tau\Delta y_j}{\dfrac{\Delta x_i}{2\lambda_{i,j}} + \dfrac{\Delta x_{i+1}}{2\lambda_{i+1,j}}} + \frac{(T^k_{i,j-1} - T^k_{i,j})\Delta\tau\Delta x_i}{\dfrac{\Delta y_j}{2\lambda_{i,j}} + \dfrac{\Delta y_{j-1}}{2\lambda_{i,j-1}}} +$$

$$+ \frac{\left(T^k_{i,j+1} - T^k_{i,j}\right)\Delta\tau\ \Delta x_i}{\dfrac{\Delta y_j}{2\lambda_{i,j}} + \dfrac{\Delta y_{j+1}}{2\lambda_{i,j+1}}} = c_{i,j}\ \rho_{i,j}\ \Delta x_i\ \Delta y_j \left(T^{k+1}_{i,j} - T^k_{i,j}\right)$$



(Fig. 5)

Finite Difference Method

Two-dimensional system (2D)

and after transformations with respect to temperature in a new time step we shall have:

$$T_{i,j}^{k+1} = T_{i,j}^{k}\left(1 - A_{i,j} - B_{i,j} - C_{i,j} - D_{i,j}\right) + A_{i,j}T_{i-1,j}^{k} + B_{i,j}T_{i+1,j}^{k} +$$

$$+ C_{i,j}T_{i,j-1}^{k} + D_{i,j}T_{i,j+1}^{k} \qquad (15)$$

where

$$A_{i,j} = \frac{2Fx_{i,j}}{1 + \dfrac{\lambda_{i,j}\Delta x_{i-1}}{\lambda_{i-1,j}\Delta x_i}} \qquad B_{i,j} = \frac{2Fx_{i,j}}{1 + \dfrac{\lambda_{i,j}\Delta x_{i+1}}{\lambda_{i+1,j}\Delta x_i}} \qquad C_{i,j} = \frac{2Fy_{i,j}}{1 + \dfrac{\lambda_{i,j}\Delta y_{j-1}}{\lambda_{i,j-1}\Delta y_j}} \qquad D_{i,j} = \frac{2Fy_{i,j}}{1 + \dfrac{\lambda_{i,j}\Delta y_{j+1}}{\lambda_{i,j+1}\Delta y_j}}$$

$$Fx_{i,j} = \frac{a_{i,j}\Delta\tau}{(\Delta x_i)^2} \qquad Fy_{i,j} = \frac{a_{i,j}\Delta\tau}{(\Delta y_j)^2} \qquad a_{i,j} = \frac{\lambda_{i,j}}{c_{i,j}\cdot\rho_{i,j}}$$

Finite Difference Method

Two-dimensional system (2D)

The stability condition of solution in equation (15) is to have:

$$A_{i,j} + B_{i,j} + C_{i,j} + D_{i,j} \leq 1$$

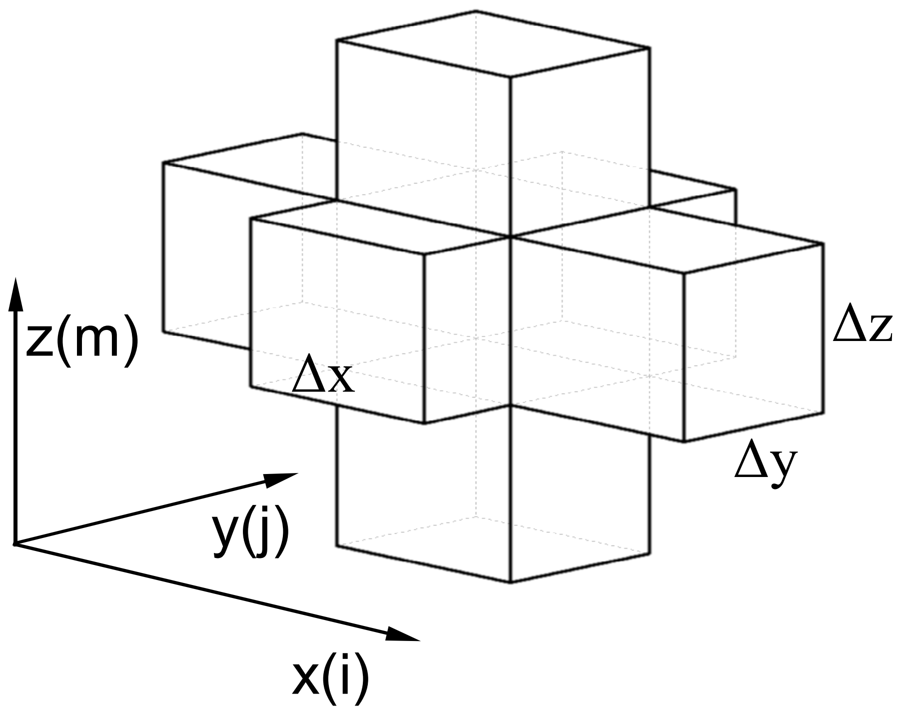
For a regular differential network ($A_{i,j} = B_{i,j} = C_{i,j} = D_{i,j} = F$), where F is the criterion determined by equation (4), the stability condition is:

$$F \leq 0.25$$

Finite Difference Method

Three-dimensional system (3D)

Compared to a 2D system, the differential equation for a 3D system can be derived by introducing to the elementary heat balance an additional balance along the axis “z” (Fig. 6)



(Fig. 6)

Finite Difference Method

Three-dimensional system (3D)

Then the differential equation will assume the form of:

$$T_{i,j,m}^{k+1} = T_{i,j,m}^{k}\left(1 - A_{i,j,m} - B_{i,j,m} - C_{i,j,m} - D_{i,j,m} - E_{i,j,m} - G_{i,j,m}\right) +$$

$$+ A_{i,j,m} T_{i-1,j,m}^{k} + B_{i,j,m} T_{i+1,j,m}^{k} + C_{i,j,m} T_{i,j-1,m}^{k} + D_{i,j,m} T_{i,j+1,m}^{k} +$$

$$+ E_{i,j,m} T_{i,j,m-1}^{k} + G_{i,j,m} T_{i,j,m+1}^{k} \qquad (16)$$

where

$$A_{i,j,m} = \frac{2Fx_{i,j,m}}{1 + \frac{\lambda_{i,j,m}\Delta x_{i-1}}{\lambda_{i-1,j,m}\Delta x_i}} \quad B_{i,j,m} = \frac{2Fx_{i,j,m}}{1 + \frac{\lambda_{i,j,m}\Delta x_{i+1}}{\lambda_{i+1,j,m}\Delta x_i}} \quad C_{i,j,m} = \frac{2Fy_{i,j,m}}{1 + \frac{\lambda_{i,j,m}\Delta y_{j-1}}{\lambda_{i,j-1,m}\Delta y_j}} \quad D_{i,j,m} = \frac{2Fy_{i,j,m}}{1 + \frac{\lambda_{i,j,m}\Delta y_{j+1}}{\lambda_{i,j+1,m}\Delta y_j}}$$

$$E_{i,j,m} = \frac{2Fz_{i,j,m}}{1 + \frac{\lambda_{i,j,m}\Delta z_{m-1}}{\lambda_{i,j,m-1}\Delta z_m}} \quad G_{i,j,m} = \frac{2Fz_{i,j,m}}{1 + \frac{\lambda_{i,j,m}\Delta z_{m+1}}{\lambda_{i,j,m+1}\Delta z_m}}$$

Finite Difference Method

Three-dimensional system (3D)

The stability condition of solution in equation (16) is to have:

$$A_{i,j,m} + B_{i,j,m} + C_{i,j,m} + D_{i,j,m} + E_{i,j,m} + G_{i,j,m} \leq 1$$

For a homogeneous system (cubic elements, the same coefficient of heat conduction), equation (16) can be written down as:

$$\mathrm{T}_{\mathrm{i,j,m}}^{\mathrm{k+1}} = \mathrm{T}_{\mathrm{i,j,m}}^{\mathrm{k}} (1 - 6\mathrm{F}) +$$

$$+ \; F \left(T_{i-1,j,m}^{k} + T_{i+1,j,m}^{k} + T_{i,j-1,m}^{k} + T_{i,j+1,m}^{k} + T_{i,j,m} + T_{i,j,m-1}^{k} + T_{i,j,m+1}^{k} \right) \qquad (17)$$

where F – Fourier's differential criterion valid for a homogeneous network.

The condition for a validility of solution in the above equation is to have $\mathrm{F} \leq 1/6$ *, which means that we have a condition three times more rigorous than the one obtained for a solution valid in 1D system.*