

Discretisation of Thermal Diffusion Equation in Multilayer Structures with Variable Material Parameters and Different Thicknesses

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Abstract. *The paper presents details of discretisation of a thermal diffusion equation in one-dimensional space in terms of the Finite Volume Method. In the following sections, the method of space discretisation is discussed along with the approximation of a spatial derivative, matrix notation of a system of equations, special cases, approximation of three types of boundary conditions and derivative approximation over time. Much attention is also given to the issue of averaging material properties which can generally be different in adjacent cells. The study aims to analyse various multilayer structures for their suitability as heat storage. The launch of studies described in the paper has been driven by the lack of methods for effective heat storage, which is currently one of the key problems faced by the renewable energy industry.*

Keywords: *heat transfer, heat storage, multilayer wall, numerical modelling, Finite Volume Method.*

1. Introduction

Flat structures composed of layers with varying material properties and different thickness through which heat passes are often encountered in technology. Such structures are found in the construction [25, 39, 46, 48], food [53], pharmaceutical [40], space [27], textile [8, 24] and other industries. Thermal analyses of multilayer structures are dominated by an analytic approach (in which the theory of thermal resistance is most commonly applied) [31], as well as the numeric approach in which numerical methods are utilised to seek solutions (Finite Difference Method [4, 6, 20, 31, 37], the Finite Element Method [17, 54, 55], the Finite Volume Method [23, 36], the Kansa Meshless Method [26] and others). It should be added that the analytic approach is mostly applied to stationary systems. For the analysis of non-stationary heat flow, when boundary conditions (e.g. ambient temperature dependent on insolation [48]), material properties (e.g. temperature-dependent heat transfer coefficient [26], or humidity-dependent material parameters [15, 50]) are changed, the numerical approach is most commonly adopted. Furthermore, in addition to standard temperature distribution analyses, the literature also refers to the works on heat storage in single- or multilayer structures [14, 29], or works analysing the acoustic properties of such structures [9]. Launching the study described in this article was driven by the former of the above mentioned trends. The objective of the study is to develop such a multilayer structure by proper selection of the number, thickness and materials of the layers that could function as heat storage. The absence of effective methods for heat storage is currently one of the key issues faced by renewable energy engineering [13, 34, 35, 52].

Numerical studies on heat transfer through various material structures have been conducted since the 1970s. The first numerical analyses referred to modelling of non-stationary heat transfer through walls with material properties constant in space and time. Over time, numerical models have gained complexity, mainly for being applied to solving new issues, requiring the taking into account of other factors affecting the processes [15, 26, 48, 50]. For quite a long time, the Finite Difference Method (FDM) has been the leading tool for solving thermal diffusion equations, and there are numerous references to this approach in literature [47, 21, 22, 30, 33, 38]. The method is still quite common, yet in recent years, there has been a growing number of works recorded in which the thermal diffusion equations are solved with the Finite Volume Method (FVM). Examples include the works of Douglas (2008) [11], Carrillo et al. (2015) [5], Bradii and Herbin (2008) [2] (in this work, the authors combine FVM with the Finite Element Method), as

well as Chandrashekar (2016) [7] (here, two different equations are solved with FVM: thermal diffusion and Navier-Stokes equations). The Finite Volume Method is distinct by the use of volume and surface balances, whereby the notion of flux has a significant role in the latter. The flux is defined as a product of any extensive value and velocity perpendicularly to a given surface. Such concept is more appropriate to diffusion processes than FDM, in which various differential analogues are referenced to equations and numerical mesh rather than directly to physics of phenomena. As a consequence, numerical modelling with FVM provides more information on the course of phenomena and processes than FDM. It should be added that the thermal diffusion equation can be solved with other methods, e.g. with the Finite Element Method, but it is still not as good a match for the physics of phenomena as is FVM.

This article presents the application concept of the Finite Volume Method (FVM) for analysing one-dimensional heat flow through multilayer structures with variable material parameters and different thickness. The reason for developing our own computational code was the observation that the available subject literature lacks descriptions of solutions to thermal diffusion equations with the Finite Volume Method. Usually, either simpler solution methods (mainly FDM) or powerful specialised software programs (e.g. ANSYS Fluent) are used. As it was feared that, in the course of time, the FDM might reveal some limitations impeding further software development, while professional numerical codes can be difficult to modify (especially those with closed source code), it was decided at the first stage to develop a proprietary computational tool. This article presents the diffusion equation in a manner typical for FVM. Furthermore, the discussion regarding the boundary and initial conditions, and the problem of variable material properties is described, and the use of so called spanning functions for creation of numerical meshes is proposed. Implementation of a thermal diffusion equation is presented in a separate article.

The motivation to write this article resulted from the difficulties in finding in literature all the information needed to write an original numerical code. Admittedly, there are works available on this issue, e.g. Desprésa (2014) [10] or Monteiro et al. (2011) [28], but they are not exhaustive and are too vague on some points to be fully useful. Therefore, it has been considered worthwhile to present a detailed and coherent derivation of numerical schemes. It should be noted that this article is of a mathematical nature, and issues concerning application of the program being developed are not covered.

2. General diffusion process equation in terms of FVM

Consider a control volume $V \in \Omega$ limited with enclosed area S . Let $\vec{\phi}$ denote a flux of physical value Φ conveyed across the area Ω . Changing the value Φ within the volume V in time dt is possible in two ways [43, 44]:

- by imbalance of the sum of fluxes $\vec{\phi}$ flowing across the area S and perpendicularly to it:

$$\delta_S = - \int_S (\vec{\phi} \cdot \vec{n}) dS, \quad (1)$$

- by action within the control volume V sources of the balanced value

$$\delta_V = \int_V s_\Phi dV, \quad (2)$$

where: \vec{n} - versor of normal direction relative to surface S (the plus sign means that the flux flows from the control volume, and the minus sign means that it flows into it); s_Φ - source of the value being balanced.

After appropriate transformations (details in [41]) we obtain the following mathematical expression:

$$\frac{\partial \Phi}{\partial t} + \text{div}(\vec{\phi}) = s_\Phi. \quad (3)$$

It is worth mentioning that the equation (3) has a very strong equivalent in fluid mechanics. If no sources are available, and the value Φ represents density of fluid ρ , the equation (3) becomes a classical mass balance equation in control volume [43]:

$$\frac{\partial \rho}{\partial t} + \text{div}(\rho \vec{v}) = 0, \quad (4)$$

where $\rho \vec{v}$ is the fluid mass flux.

If the flux $\vec{\phi}$ is proportional to value gradient Φ , then (3) will take the form:

$$\frac{\partial \Phi}{\partial t} + \text{div}(-\alpha \cdot \nabla \Phi) = s_\Phi \quad (5)$$

or

$$\frac{\partial \Phi}{\partial t} - \alpha \cdot \nabla^2 \Phi = s_\Phi, \quad (6)$$

where α is the proportionality factor.

Depending on physical interpretation, the equation (6) can describe various processes with diffusive character, for example the heat flow. Substituting Fourier's law [1, 3, 12, 19, 49] for equation (6):

$$\vec{q}_T = -\lambda \cdot \nabla T, \quad (7)$$

where: \vec{q}_T - density of heat flux perpendicularly to the surface across which the heat flows [W/m^2], λ - heat transfer coefficient [$W/(m \cdot K)$], ∇T - temperature gradient [K/m]; so called thermal diffusion equation will be obtained:

$$\frac{\partial T}{\partial t} - \lambda \cdot \nabla^2 T = s_T, \quad (8)$$

where s_T is the source of heat [K/s].

Another example of a process with the same physical mechanism is the phenomenon of component diffusion in a mixture. Substituting for equation (6) the Fick's first law [16, 49, 56]:

$$\vec{j}_C = -D \cdot \nabla C, \quad (9)$$

where: \vec{j}_C - amount of substance flowing through the unitary cross section in a unit of time [$mol/(m^2 \cdot s)$], D - diffusion factor [m^2/s], ∇C - substance concentration gradient [mol/m^4]; the equation takes the form:

$$\frac{\partial C}{\partial t} - D \cdot \nabla^2 C = s_C, \quad (10)$$

where s_C is the source of component concentration [$mol/(m^2 \cdot s)$].

Similarly, by means of the general equation (6), other processes can be expressed, such as electrical media flow in semiconductors, or Markov processes. The discussion that follows applies exclusively to the thermal diffusion equation.

3. Boundary and initial conditions of a numerical solution

One-dimensional heat flow through a flat homogeneous structure is described in the literature with the aid of a parabolic differential partial equation [4, 6, 20, 31]:

$$\frac{\partial T}{\partial t} - \frac{\partial}{\partial x} \left(\frac{\lambda}{c_p \rho} \frac{\partial T}{\partial x} \right) = S(t, x), \quad (11)$$

for $x \in [x_A, x_B]$ and $t \in [0, t_k]$, where: $T(t, x)$ - temperature [$^{\circ}C$], t - time [s], t_k - end time [s], x - spatial coordinate [m], λ - heat transfer coefficient [$W/(m \cdot K)$], c_p - material specific heat [$J/(kg \cdot K)$], ρ - material density [kg/m^3]. Function $S(t, x)$ represents additional internal heat sources [K/s].

The equation (11) is an equivalent of the expression (8), yet the heat transfer coefficient has been replaced with the temperature balance factor, also taking into consideration the material density and specific heat. This action is essential to analyse changes of heat accumulated in individual areas (cells of numerical grid) rather than only the temperature distribution.

In a general case, the material parameters can depend on both the location (heterogeneous structure) and time (degrading structure), then $\lambda = \lambda(t, x)$, $c_p = c_p(t, x)$ and $\rho = \rho(t, x)$. Further in the article the material parameters are denoted with an overall symbol $D = D(t, x)$. The dimension of that component is [m^2/s].

To provide an unambiguous solution to the equation (11) it is necessary to determine the initial condition:

$$T(0, x) = T_0(x), \quad (12)$$

where $T_0(x)$ is a known function, and boundary conditions valid in points x_A and x_B at any time $t \in [0, t_x]$.

To ensure the universality of the solution, various types of boundary conditions have to be introduced (they are provided for x_A ; for x_B defined accordingly). In further solutions, it is proposed to consider:

- a) The Dirichlet condition defining temperature value at the wall end

$$T(t, x_A) = T_A(t). \quad (13)$$

- b) The Neumann condition defining heat flux passing through the wall in time

$$\frac{\lambda}{c_p \rho} \frac{\partial T}{\partial x} \Big|_A = F_A(t), \quad (14)$$

where $F_A(t)$ is the heat flux reaching the wall at the point x_A .

- c) The mixed condition determining the relationship between the flux passing through the wall in time t and outside temperature difference T_{in} , temperature at

the wall edge T_A and loss (described with the factor α) while passing through the wall edge

$$\frac{\lambda}{c_p \rho} \frac{\partial T}{\partial x} \Big|_A = \alpha(T_A(t) - T_{in}(t)). \quad (15)$$

4. Problem of variable material parameters

Differential equation (11) can be solved numerically. Historically, the first such solution was achieved using the Finite Difference Method, in which the derivatives are replaced with appropriate finite difference schemes, based on the values determined in the subsequent nodes of the mesh [1, 18, 51]. Such a scheme, written for one axis of a coordinate system, can take the form:

$$\frac{T_i^{t+\Delta t} - T_i^t}{\Delta t} + \frac{\lambda}{c_p \rho} \frac{-T_{i-1}^t + 2T_i^t - T_{i+1}^t}{(\Delta x)^2} = 0, \quad (16)$$

where: i - node number [-], t - time [s], Δt - time step [s], Δx - spatial step [m].

However, the scheme (16) is not suitable for modelling multilayer structures, as it is insensitive to the spatial variability of material parameters λ , c_p and ρ . Regardless of what values are taken by the parameters in individual nodes or cells of the mesh, the solution always tends to the linear form which, for instance, for multilayer walls, is opposite to the observations. Patankar (1980) [32] proposed to solve that problem by the application of harmonic weighted averaging of material characteristics. Kadioglu et al. (2008) [20] proposes the use of arithmetic weighted averaging, and demonstrates that in some instances it is more favourable than harmonic averaging. The indications provided in the cited works relate to solutions based on the Finite Difference Method, yet they can be used to develop a numerical scheme conforming to the Finite Volume Method concept. This issue is described further.

5. The problem of variable thickness of the layers

The discussion presented in the works of Patankar and Kadioglu et al. refers to regular meshes, i.e. with fixed spatial steps. This solution performs well in the case of structures composed of layers with comparable thicknesses. When the layer thickness differences are significant, the mesh has to be generated so as to enable

proper action of the numerical scheme in the thinnest layer. This condition might require building meshes composed of tens or hundreds of thousands of cells. Regrettably, the larger the number of mesh cells, the greater the computer RAM and computing power required.

A solution to the above issue can be the use of so called spanning functions which control the distribution of the mesh nodes and their local concentration. Such functions are used as a standard in numerical fluid mechanics for modelling phenomena occurring at the wall layer, where the fluid viscosity is of critical importance, or for the modelling of issues related to impact waves. The most commonly used spanning functions include:

a) linear function (Fig. 1 example 1): $f = \frac{i-1}{N-1}$,

b) exponential function (Fig. 1 example 2): $f = \frac{\exp\left(\alpha \frac{i-1}{N-1}\right) - 1}{\exp(\alpha) - 1}$,

c) hyperbolic tangent based function (Fig. 1 example 3): $f = 1 + \frac{\tanh\left(\alpha \left(\frac{i-1}{N-1} - 1\right)\right)}{\tanh(\alpha)}$,

d) hyperbolic sine based function (Fig. 1 example 4): $f = \frac{\sinh\left(\alpha \frac{i-1}{N-1}\right)}{\sinh(\alpha)}$.

Symbols in the equations denote, respectively: N - number of nodes, i - current node number, α - node distribution control factor.

To calculate the coordinates of individual boundary points, use the following formula:

$$x_i = f x_A + (1 - f) x_B, \quad (17)$$

where: x_i - node coordinate [m], x_A - mesh start (first node) coordinate [m], x_B - mesh end (last node) coordinate [m].

Figure 1 shows distribution examples of mesh nodes obtained from the four above mentioned spanning functions. In addition to the linear function case, the distribution is asymmetric. To achieve symmetry in the node distribution of each layer of the wall, it has to be divided into halves and the equation (17) applied, whereby to calculate the coordinates of nodes in the first half of the wall, the variables x_A and x_B have to swap positions. The method works when the number of nodes is greater than three.

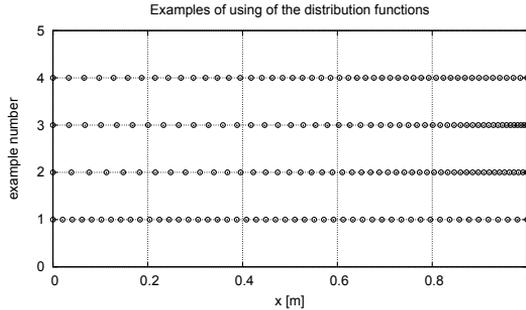


Figure 1: Example of mesh node distribution ($\alpha = 1.5$)

6. Space discretisation - basis of the numerical scheme

The majority of methods for numerical solution of partial differential equations are based on nodes distinguished in calculation space (in this case, it is the section $[x_A, x_B]$) and on cells or elements built on them (naming is usually related to a specific numerical method).

An example of discretisation of a one-dimensional space (section $[x_A, x_B]$) consistent with the Finite Volume Method [43, 44] can be seen in Fig 2. The nodes are denoted x_i^n , where $i = 1, \dots, N$. The symbol x_i^c , where $i = 1, \dots, M$, ($M = N - 1$), can be identified with central points of computational cells built on the basis of nodes or with entire cells. x_i^c specifically signifies the section $[x_i^n, x_{i-1}^n]$. This is a one-dimensional representation of finite (or control) volume, for which balance equations are composed in FVM. Still, the superscripts n signify references to nodes, and superscripts c denote cells (identified with their central points). Δx_i^n signifies the distance between nodes x_i^n and x_{i+1}^n , while Δx_i^c denotes the distance between centres of adjacent cells, x_i^c and x_{i+1}^c . Further in the paper, to simplify the notation, the expressions "cell i " (Fig. 2) and "node i " are used (always the node on the left side of the cell i).

7. Numerical solution to a heat transfer equation

The equation (11) is considered in the form:

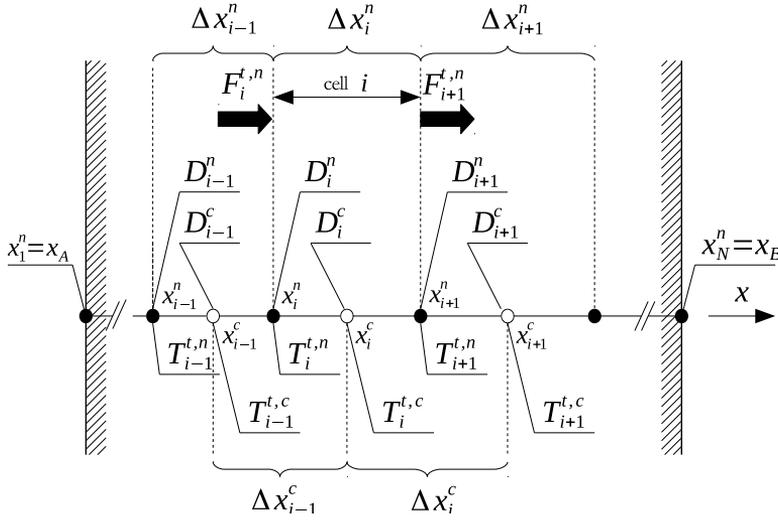


Figure 2: Symbols used in numerical schemes

$$\frac{\partial T}{\partial t} - \frac{\partial F}{\partial x} = 0, \quad (18)$$

where

$$F = \frac{\lambda}{c_p \rho} \frac{\partial T}{\partial x} \quad (19)$$

is the heat flux. For an equation in this form, the approximation scheme will be derived.

In the initial consideration, for the sake of simplicity, we assume a steady-state case and equation contains no evolution component:

$$-\frac{\partial}{\partial x} \left(\frac{\lambda}{c_p \rho} \frac{\partial T}{\partial x} \right) = 0, \quad (20)$$

for $x \in [x_A, x_B]$ and $t \in [0, t_k]$.

Using the flux of heat (19), we consider the equation in the form:

$$-\frac{\partial F}{\partial x} = 0. \quad (21)$$

Boundary conditions will be taken into account later.

8. Approximation of spatial derivative

Based on discretisation of computational domain (Fig. 2), derivative $\partial F/\partial x$ in the cell i can be expressed in the form of surface balance typical for FVM, here in a 1D form:

$$\left. \frac{\partial F}{\partial x} \right|_i \cong \frac{F_{i+1}^{t,n} - F_i^{t,n}}{\Delta x_i^n}. \quad (22)$$

$F_i^{t,n}$ denotes the flux of heat flowing into the cell (through a node with the coordinate x_i^n), while $F_{i+1}^{t,n}$ is the flux of heat leaving it (through a node with the coordinate x_{i+1}^n), and symbol t represents the point in time. As a consequence of the assumption that there are no heat sources present in this case, both fluxes have to be equal.

In the subsequent step, when replacing the derivative $\partial T/\partial x$ in the equation (19) with the differential quotient, a representation of the flux $F_i^{t,n}$ is obtained in the form of the following differential scheme:

$$F_i^{t,n} = D_i^n \frac{T_i^{t,c} - T_{i-1}^{t,c}}{\Delta x_{i-1}^c}. \quad (23)$$

Terms of the equation (23) require commentary. Note that to determine a discrete value of a flux in the node i , temperature values T in the cells around that node are used, namely the cells $i-1$ and i (Fig. 2). As previously mentioned, the discrete temperature T can be interpreted as a value in a central point of the cell $T_i^{t,c}$. It can be understood that the temperature is constant in the entire cell. Similarly, material parameters of the centre λ , c_p and ρ and an auxiliary coefficient D refer to cell (hence indices c):

$$D_i^c = \frac{\lambda^c}{c_p^c \rho^c}. \quad (24)$$

Meanwhile, the index n in the coefficient D_i^n in (23) means that represents the material properties in the node i . Therefore, its value depends on the material parameters of the both adjacent cells:

$$D_i^n = f\left(\frac{\lambda_{i-1}^c}{c_{p,i-1}^c \rho_{i-1}^c}, \frac{\lambda_i^c}{c_{p,i}^c \rho_i^c}\right). \quad (25)$$

Most commonly, weighted averaging is used as f [20, 32]: harmonic or arithmetic.

For a harmonic weighted average, the value of parameter D_i^n is expressed as:

$$D_{i,harm}^n = \frac{\Delta x_{i-1}^n + \Delta x_i^n}{\frac{\Delta x_{i-1}^n}{D_{i-1}^c} + \frac{\Delta x_i^n}{D_i^c}}. \quad (26)$$

For the arithmetic weighted average, it yields:

$$D_{i,aryt}^n = \frac{\Delta x_{i-1}^n D_{i-1}^c + \Delta x_i^n D_i^c}{\Delta x_{i-1}^c + \Delta x_i^c}. \quad (27)$$

Similarly, the representation of a flux passing through the second edge is determined as:

$$F_{i+1}^{t,n} = D_{i+1}^n \frac{T_{i+1}^{t,c} - T_i^{t,c}}{\Delta x_i^c}. \quad (28)$$

Taking into account the relationships (23) and (28), the approximation (22) takes the form of:

$$\left. \frac{\partial F}{\partial x} \right|_i \cong \frac{F_{i+1}^{t,n} - F_i^{t,n}}{\Delta x_i^n} = D_{i+1}^n \frac{T_{i+1}^{t,c} - T_i^{t,c}}{\Delta x_i^c \Delta x_i^n} - D_i^n \frac{T_i^{t,c} - T_{i-1}^{t,c}}{\Delta x_{i-1}^c \Delta x_i^n}, \quad (29)$$

where D_i^n and D_{i+1}^n stand for harmonic (26) or arithmetic (27) averages.

The relationship (29) in the case of homogeneous structures, or in the case of a uniform division of the space into cells, is simplified. This will be presented further in the paper.

The relationship (29) has to be fulfilled in all computational cells, and therefore, substituting (29) for (21), or the entire numerical mesh, not a single equation, but a system of equations is obtained:

$$\frac{F_{i+1}^{t,n} - F_i^{t,n}}{\Delta x_i^n} = D_{i+1}^n \frac{T_{i+1}^{t,c} - T_i^{t,c}}{\Delta x_i^c \Delta x_i^n} - D_i^n \frac{T_i^{t,c} - T_{i-1}^{t,c}}{\Delta x_{i-1}^c \Delta x_i^n} = 0, \quad (30)$$

for $i = 2, \dots, M - 1$, where M is the number of mesh cells.

Arranging components with respect to temperatures in individual cells, the system of equations (30) transforms into:

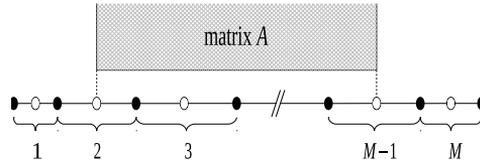


Figure 3: Cell numbering and matrix index range scheme

$$-\frac{D_i^n}{\Delta x_{i-1}^c \Delta x_i^n} T_{i-1}^{t,c} + \left[\frac{D_i^n}{\Delta x_{i-1}^c \Delta x_i^n} + \frac{D_{i+1}^n}{\Delta x_i^c \Delta x_i^n} \right] T_i^{t,c} - \frac{D_{i+1}^n}{\Delta x_i^c \Delta x_i^n} T_{i+1}^{t,c} = 0, \quad (31)$$

for $i = 2, \dots, M - 1$. Note that ((30) and ((31) do not include schemes for the extreme cells $i = 1$ and $i = M$. Their definition requires taking into account the boundary conditions, which will be given further explanation in later sections. For the time being, we should assume that these schemes are also known.

9. Discretization scheme in a matrix form

A sequence of equations (31) can be presented in a matrix form as a system of linear equations:

$$A \cdot T = B. \quad (32)$$

Due to the construction method, A is a tridiagonal matrix, the dimension of which depends on the number of cells M as well as on the type of boundary conditions adopted (Fig. 3):

- a) If, on two edges, Dirichlet conditions are assumed, then the number of unknowns equals $M - 2$ (the number of cells reduced by two known solutions in the first and last cell of the mesh), and the size of matrix A will be $(M - 2) \times (M - 2)$;
- b) If, on one of the edges, the Dirichlet condition is assumed and the Neumann or mixed condition on the other, then the number of unknowns will increase by 1, and the size of matrix A will be $(M - 1) \times (M - 1)$;
- c) If, on two edges, the Neumann or mixed condition is defined, then the number of unknowns will equal the number of cells in the space, and the size of matrix A will be $M \times M$.

Further in the paper, it is assumed that elements of the matrix A are indexed from 2 to $M-1$. Additional unknowns, created by imposing the Neumann or mixed condition, are determined explicitly based on temperature values from the previous time step. Such an approach does not deteriorate the quality of the solution, but it is much more convenient to implement.

Non-zero elements of the matrix A on the diagonal (elements $A_{i,i}$) equal to

$$A_{i,i} = \left(\frac{D_i^n}{\Delta x_{i-1}^c} + \frac{D_{i+1}^n}{\Delta x_i^c} \right) \frac{1}{\Delta x_i^n}, \quad (33)$$

for $i = 2, \dots, M-1$; under the diagonal (elements $A_{i,i-1}$)

$$A_{i,i-1} = -\frac{D_i^n}{\Delta x_{i-1}^c} \frac{1}{\Delta x_i^n}, \quad (34)$$

for $i = 2, \dots, M-1$; and over the diagonal (elements $A_{i,i+1}$)

$$A_{i,i+1} = -\frac{D_{i+1}^n}{\Delta x_i^c} \frac{1}{\Delta x_i^n}, \quad (35)$$

for $i = 2, \dots, M-1$.

Other elements A equal zero. Such matrix structure results from the fact that every differential scheme (31) combines the temperatures assigned to three adjacent cells only.

The (column) vector T includes the unknown temperatures T_i^c . B denotes the (column) vector of the right hand side with elements B_i^c . The superscript c means that vectors elements are linked to the cells. In a general case, the size of vectors T and B also depends on the type of boundary conditions imposed; here however, since a constant size of the matrix A is assumed, this will equal $M-2$.

While in the space there are no sources, the elements of the vector B , except possibly for the first and last elements, equal zero. In the case of heat sources present in the domain, their performance is expressed in the scheme by non-zero elements B_i^c of the vector B .

10. Special cases

The scheme discussed in the previous section, and the resulting form of the matrix A , refers to the most general case, significant in the context of the problem being solved. Several special cases can be distinguished.

Case 1 - nodes distributed uniformly, various values of material parameters. As in this case $\Delta x_i^c = \Delta x_{i-1}^c = \Delta x_i^n = \Delta x_{i-1}^n = \dots$, the formulas describing elements of the matrix A are simplified:

$$A_{i,i} = \frac{D_i^n + D_{i+1}^n}{(\Delta x)^2}, A_{i,i-1} = -\frac{D_i^n}{(\Delta x)^2}, A_{i,i+1} = -\frac{D_{i+1}^n}{(\Delta x)^2}. \quad (36)$$

The formulas for the averaged values of the coefficient D will also be simplified:

$$D_{i,harm}^n = \frac{\Delta x + \Delta x}{\frac{\Delta x}{D_{i-1}^c} + \frac{\Delta x}{D_i^c}} = \frac{2D_{i-1}^c D_i^c}{D_i^c + D_{i-1}^c}, D_{i,aryt}^n = \frac{D_{i-1}^c + D_i^c}{2}. \quad (37)$$

Case 2 - non-uniformly distributed nodes, constant value of the parameter D (homogeneous case):

$$A_{i,i} = \left(\frac{1}{\Delta x_{i-1}^c} + \frac{1}{\Delta x_i^c} \right) \frac{D}{\Delta x_i^n}, A_{i,i-1} = -\frac{D}{\Delta x_{i-1}^c} \frac{1}{\Delta x_i^n}, A_{i,i+1} = -\frac{D}{\Delta x_i^c} \frac{1}{\Delta x_i^n}. \quad (38)$$

Case 3 - uniformly distributed nodes, constant value of the parameter D :

$$A_{i,i} = \frac{2D}{(\Delta x)^2}, A_{i,i-1} = -\frac{D}{(\Delta x)^2}, A_{i,i+1} = -\frac{D}{(\Delta x)^2}. \quad (39)$$

In this case, the matrix A takes the form:

$$A = \frac{D}{\Delta x^2} \begin{pmatrix} 2 & -1 & 0 & \dots & 0 \\ -1 & 2 & -1 & \dots & \dots \\ 0 & -1 & 2 & \dots & 0 \\ \dots & \dots & \dots & \ddots & -1 \\ 0 & \dots & 0 & -1 & 2 \end{pmatrix}. \quad (40)$$

This form is most commonly found in literature [1, 18, 38, 41, 51] in terms of the Finite Difference Methods. In this special case, the equivalent of the scheme (31) has the form:

$$-\frac{D}{\Delta x^2} T_{i-1}^{t,c} + \frac{2D}{\Delta x^2} T_i^{t,c} - \frac{D}{\Delta x^2} T_{i+1}^{t,c} = 0, \quad (41)$$

where $i = 2, \dots, M - 1$.

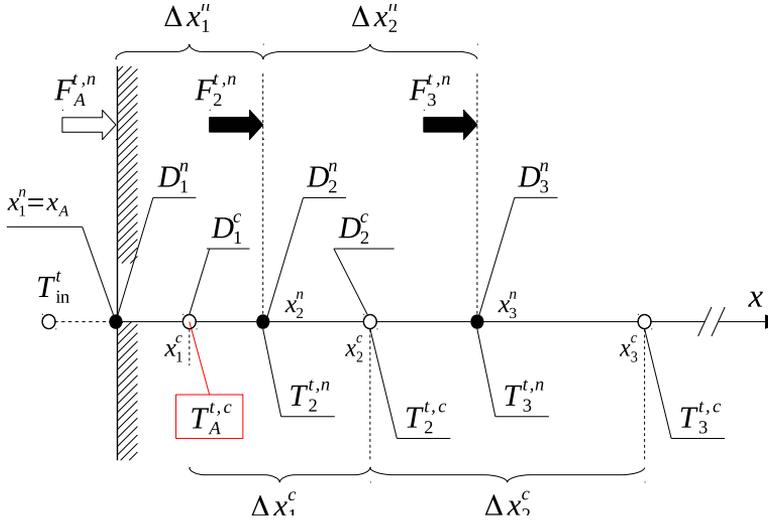


Figure 4: Scheme of a numerical mesh at the left wall edge

11. Approximation of boundary conditions

The boundary conditions have to be taken into account in the numerical scheme. They affect the value of the first (index 2) and last (index $M - 1$) element of the matrix A and the first and last element of the right hand side vector B . Similarly, as in the case of the matrix A , it is further assumed that the elements of vectors B and T are indexed from 2 to $M - 1$. Therefore, consistency is maintained between the indices of matrix and vector elements and cell numbering.

Dirichlet boundary condition. When imposing the Dirichlet condition (Eq. 13), it is assumed that the temperature value in the first cell is known and is $T_A^{t,c}$ (vector $T^{t,c}$ has no element with index 1, hence the new symbol; similarly, further in the paper, the symbol $T_B^{t,c}$ is introduced, which denotes the temperature in the last cell of the mesh). The scheme (30) for the second cell takes the form (Fig. 4):

$$\frac{F_3^{t,n} - F_2^{t,n}}{\Delta x_2^n} = D_3^n \frac{T_3^{t,c} - T_2^{t,c}}{\Delta x_2^c \Delta x_2^n} - D_2^n \frac{T_2^{t,c} - T_A^{t,c}}{\Delta x_1^c \Delta x_2^n} = 0. \quad (42)$$

After arranging with respect to temperatures, the first equation of the system of equations (31) is obtained:

$$\left[\frac{D_2^n}{\Delta x_1^c \Delta x_2^n} + \frac{D_3^n}{\Delta x_2^c \Delta x_2^n} \right] T_2^{t,c} - \frac{D_3^n}{\Delta x_2^c \Delta x_2^n} T_3^{t,c} = \frac{D_2^n}{\Delta x_1^c \Delta x_2^n} T_A^{t,c}. \quad (43)$$

The right side of the equation (43) constitutes the first element (with index 2) of the vector B^c :

$$B_2^c = \frac{D_2^n}{\Delta x_1^c \Delta x_2^n} T_A^{t,c}. \quad (44)$$

In the special case of a zero boundary condition ($T_A^{t,c} = 0$) $B_2^c = 0$.

On the right hand site of the domain, the equations (42) and (43) take the form:

$$\frac{F_{N-1}^{t,n} - F_{N-2}^{t,n}}{\Delta x_{M-1}^n} = D_{N-1}^n \frac{T_B^{t,c} - T_{M-1}^{t,c}}{\Delta x_{M-1}^c \Delta x_{M-1}^n} - D_{N-2}^n \frac{T_{M-1}^{t,c} - T_{M-2}^{t,c}}{\Delta x_{M-2}^c \Delta x_{M-1}^n} = 0 \quad (45)$$

and

$$-\frac{D_{N-2}^n}{\Delta x_{M-2}^c \Delta x_{M-1}^n} T_{M-2}^{t,c} + \left[\frac{D_{N-2}^n}{\Delta x_{M-2}^c \Delta x_{M-1}^n} + \frac{D_{N-1}^n}{\Delta x_{M-1}^c \Delta x_{M-1}^n} \right] T_{M-1}^{t,c} = \frac{D_{N-1}^n}{\Delta x_{M-1}^c \Delta x_{M-1}^n} T_B^{t,c}, \quad (46)$$

where $T_B^{t,c}$ is the known temperature value in the last cell of the mesh.

Therefore, the last element of the vector B^c (with index $M - 1$) takes the form:

$$B_{M-1}^c = \frac{D_{N-1}^n}{\Delta x_{M-1}^c \Delta x_{M-1}^n} T_B^{t,c}. \quad (47)$$

In the special case of a zero boundary condition ($T_B^{t,c} = 0$) $B_{M-1}^c = 0$.

Neumann boundary condition. In case of the Neumann condition (Eq. 14), it is assumed that the value of the heat flux passing through the wall edge is known. Therefore, the balance of heat fluxes for the first cell (finite volume) takes the form (Fig. 5):

$$F_A^{t,n} = F_2^{t,n} = D_2^n \frac{T_2^{t,c} - T_A^{t,c}}{\Delta x_1^2}, \quad (48)$$

whereby, according to the concept adopted in this paper, for value $T_2^{t,c}$, the temperature from the previous time step is substituted.

After transformation, the temperature value in the first cell is:

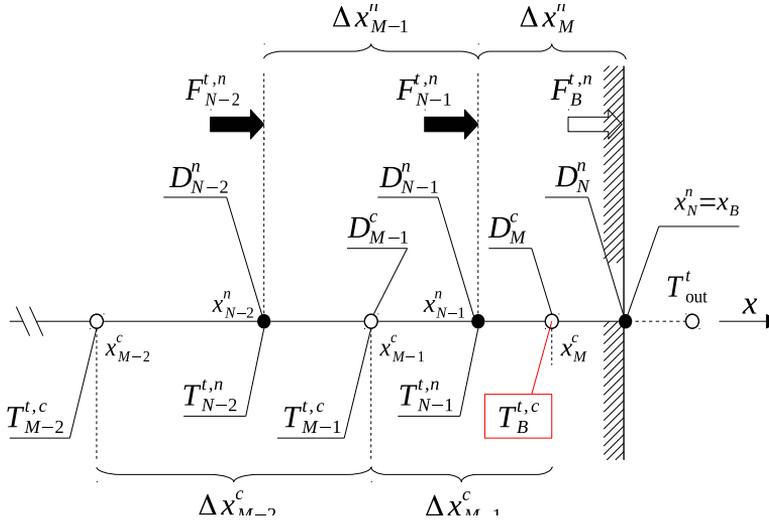


Figure 5: Scheme of a numerical mesh at the right wall edge

$$T_A^{t,c} = T_2^{t,c} - F_A^{t,n} \frac{\Delta x_1^c}{D_2^n}. \quad (49)$$

Particularly for $F_A^{t,n} = 0$ (insulated wall edge), this yields: $T_A^{t,c} = T_2^{t,c}$.
The analogical formula for the last cell of the mesh can be defined as:

$$F_{N-1}^{t,n} = D_{N-1}^n \frac{T_{M-1}^{t,c} - T_B^{t,c}}{\Delta x_{M-1}^c} = F_B^{t,n}. \quad (50)$$

Therefore:

$$T_B^{t,c} = T_{M-1}^{t,c} - \frac{F_B^{t,c}}{D_{N-1}^n} \Delta x_{M-1}^c. \quad (51)$$

Particularly for $F_B^{t,n} = 0$ (isolated domain), this yields: $T_B^{t,c} = T_{M-1}^{t,c}$.

Mixed boundary condition. The mixed boundary condition (Eq. 15) relates the value of the (unknown) temperature in the extreme cell of the domain and the (known external) temperature outside the domain to the heat flux passing through that boundary.

To describe the heat flux flowing from the outside to the inside (centre) of the first cell of the mesh, Newton's law of cooling can be applied [42]:

$$q_N = \alpha_{in} \Delta T \quad (52)$$

or, in the case in question:

$$q_N = \alpha_{in}(T_{in}^t - T_A^{t,c}). \quad (53)$$

The heat absorption coefficient α_{in} [$W/(m^2 \cdot K)$] is a parameter dependent upon the types of materials, including the layers between which heat is absorbed, and upon the conditions present at the interface of the layers.

The flux of heat transferred from the first to the second cell of the mesh can be presented in accordance with the Fourier law [42]:

$$q_F = -\lambda \frac{\partial T}{\partial x}, \quad (54)$$

which is discretised for the computational mesh in the form:

$$q_F = \lambda \frac{T_A^{t,c} - T_2^{t,c}}{\Delta x_1^c}. \quad (55)$$

The heat transfer coefficient λ [$W/(m \cdot K)$] is a material feature and generally represents the function of temperature. To maintain consistency with the physical model presented above, instead of the coefficient λ , the more general material parameter D is applied.

Since both fluxes have to be equal, the equations (53) and (55) can be equated by sides:

$$\alpha_{in}(T_{in}^t - T_A^{t,c}) = D_2^n \frac{T_A^{t,c} - T_2^{t,c}}{\Delta x_1^c} \quad (56)$$

From that point, the formula for temperature in the first cell of the mesh can be determined as:

$$T_A^{t,c} = \frac{\alpha_{in} \Delta x_1^c T_{in}^t + D_2^n T_2^{t,c}}{\alpha_{in} \Delta x_1^c + D_2^n}. \quad (57)$$

Here, also for the value $T_2^{t,c}$, the temperature from the previous time step is substituted.

The flux flowing from inside of the domain to the last cell of the mesh can be defined accordingly:

$$q_F = D_{N-1}^n \frac{T_{M-1}^{t,c} - T_B^{t,c}}{\Delta x_{M-1}^c} \quad (58)$$

and then outside:

$$q_N = \alpha_{out}(T_B^{t,c} - T_{out}^t). \quad (59)$$

After equating the right sides of both equations and performing such transformations as before, the formula for the temperature in the last cell of the mesh will be obtained:

$$T_B^{t,c} = \frac{D_{N-1}^n T_{M-1}^{t,c} + \alpha_{out} \Delta x_{M-1}^c T_{out}^t}{D_{N-1}^n + \alpha_{out} \Delta x_{M-1}^c}. \quad (60)$$

12. Time discretization

Up to now, except for explicit boundary conditions, we have not discussed the issue of evolution of the modelled phenomenon in time. The superscripts at the variables t denoted references to a certain (discrete) moment of time t .

The time interval encompassing the process of the phenomenon being studied has to be discretised by dividing the time span $[0, t_k]$ into sections equal in length to the time step Δt . Within the framework of this work, we assume a constant time step for a given simulation.

Approximation of a time derivative in the Eq. (11) with a differential quotient spanned over discretization time step, is expressed with the formula:

$$\frac{\partial T}{\partial t} \approx \frac{T_i^{t+\Delta t,c} - T_i^{t,c}}{\Delta t}. \quad (61)$$

Having substituted the equations (61) and (30) for (18), a full approximation of the equation (11) will be obtained:

$$\frac{T_i^{t+\Delta t,c} - T_i^{t,c}}{\Delta t} - \left[D_{i+1}^n \frac{T_{i+1}^{t,c} - T_i^{t,c}}{\Delta x_i^c \Delta x_i^n} - D_i^n \frac{T_i^{t,c} - T_{i-1}^{t,c}}{\Delta x_{i-1}^c \Delta x_i^n} \right] = 0 \quad (62)$$

for $i = 2, \dots, M - 1$.

This equation can be presented more generally as:

$$CT^{t+\Delta t,c} - CT^{t,c} + AT^{*,c} = B^c, \quad (63)$$

where $T^{*,c}$ denotes the temperature vector for the time step t or $t + \Delta t$, depending on the method of calculations in time further adopted. C is a matrix with the same dimensions as the matrix A , having non-zero elements with the value $1/\Delta t$ only on the diagonal.

By substituting $T^{*,c} = T^{t,c}$, an explicit scheme is obtained, and every temperature distribution in a next time step is calculated based only on the temperature history. For the first time step, a table of initial values $T^{t=0,c}$ (initial condition) is required. Since these are diagonal matrices, it is sufficient to solve the equation:

$$T^{t+\Delta t,c} = \Delta t(CT^{t,c} - AT^{t,c} + B^c). \quad (64)$$

It must be emphasized that the explicit scheme is conditionally stable, whereby the limitation refers to the relationship of the maximum permissible time step in combination with the size of the spatial mesh.

$$\Delta t \leq \frac{1}{2}D(\Delta x)^2. \quad (65)$$

In the case of irregular meshes, the length of the smallest cell should be considered as Δx .

If $T^{*,c} = T^{t+\Delta t,c}$ is adopted, the following implicit scheme is obtained:

$$CT^{t+\Delta t,c} - CT^{t,c} + AT^{t+\Delta t,c} = B^c. \quad (66)$$

After transformations, the following system of equations is obtained:

$$(C + A)T^{t+\Delta t,c} = B^c + CT^{t,c}. \quad (67)$$

Another option is to use the Crank-Nicolson scheme (semi-explicit and semi-implicit). In such a case:

$$CT^{t+\Delta t,c} - CT^{t,c} + \frac{1}{2}AT^{t,c} + \frac{1}{2}AT^{t+\Delta t,c} = B^c. \quad (68)$$

Regardless of the approach to the solution of equation in the time provided, the matrices and vectors in individual formulas are the same.

From the technical point of view, the fundamental difference between the explicit and implicit schemes is the necessity to solve (linear) systems of equations

for the implicit schemes. In the case of explicit schemes, solutions in the following time step are determined independently for each point (cell).

13. Summary

The following recommendation could be formulated for further implementation of the presented numerical schemes:

1. An equation of any diffusion process can be written in a form typical to the Finite Volume Method.

2. The application of the Finite Volume Method appears to be very favourable for its being well matched to the physics of diffusion processes in which the fluxes of balanced values play the key role.

3. The application of spanning functions for the creation of numerical meshes should noticeably influence the performance of the computational code, particularly in the case of structures comprising layers with significantly different thicknesses.

4. Creating and using independent computational software seems to be the optimum solution due to the full control of all calculation aspects, in particular the possibility of any modification of the mathematical model and calculation procedures.

5. Developing detailed numerical schemes requires an accurate definition of indices of individual table variables. Figures presenting the computational mesh in the centre and at the edges of the space being modelled have proven to be of great help.

6. The description of numerical schemes and implementation in a selected programming language have to be performed simultaneously. Therefore, it will be relatively easy to discover errors in the program or in its description.

7. In the implementation of differential equations, good planning of the names of variables and constants present in the program is of high practical importance. They should correspond to the symbolism used in the description and refer to the nature of the tasks being completed. Relevant figures are also very helpful at this stage.

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