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DESIGN OPTIMIZATION OF A HEAT EXCHANGER WITH A PHASE CHANGE MATERIAL FOR THERMAL ENERGY STORAGE

OPTIMALIZACE NÁVRHU TEPELNÉHO VÝMĚNÍKU VYUŽÍVAJÍCÍ MATERIÁL SE ZMĚNOU FÁZE PRO AKUMULACI TEPLA

MASTER'S THESIS
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Pursuant to Act no. 111/1998 concerning universities and the BUT study and examination rules, you have been assigned the following topic by the institute director Master's Thesis:

Design optimization of a heat exchanger with a phase change material for thermal energy storage

Concise characteristic of the task:

Heat transfer with phase changes takes place in a number of engineering applications. Recently, latent heat thermal energy storage (LHTES) has attracted an attention of researchers and investigators. A solar air heat exchanger is an LHTES device which enables the utilization of solar energy. An optimal design and setup of the heat exchanger significantly influence its use and performance.

Goals Master's Thesis:

The diploma thesis aims at the development of the computer model of the solar air heat exchanger, which is assembled of commercially available containers filled with a phase change material. The numerical model will further be used in the optimization model, which will be implemented in an appropriate software. The main aim of the thesis is to perform an optimization analysis of the heat exchanger for the determination of optimal design and operational parameters.

Recommended bibliography:

RAO, Singiresu S. Engineering optimization: Theory and practice. 4th ed. Hoboken: Wiley, 2009. ISBN 978-0-470-18352-6.

STEFANESCU, Doru. Science and engineering of casting solidification. 2nd ed. New York: Springer, 2009. ISBN 978-144-1945-099.

INCROPERA, Frank P., David P. DEWITT, Theodore L. BERGMAN and Adrienne S. LAVINE. Principles of heat and mass transfer. 7th ed. Singapore: John Wiley, 2013. ISBN 978-0-470-64615-1.

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Summary
This diploma thesis is focused on the development of the computer model of the thermal energy storage unit with an appropriate phase change material. Furthermore, this model is used for a design optimization aimed to the maximization of the stored heat. Due to the complexity of the objective function a suitable genetic algorithm is chosen to solve design optimization problems. Two design optimization problems are analysed and obtained results are presented and discussed. The complete problem was implemented in Matlab.

Abstrakt
Práce je zaměřena na sestavení numerického modelu akumulace tepelné energie s fázovou přeměnou. Následně je tento model použit při tvarové optimalizaci, jejíž cílem je maximalizace uloženého tepla v tepelném výměníku. Kvůli komplexitě objektové funkce byl zvolen genetický algoritmus pro řešní úloh tvarové optimalizace. Práce obsahuje analýzu dvou problému týkající se tvarové optimalizace s následnou diskuzí nad obdrženými výsledky. Celý problém byl implementován v softwaru Matlab.

Keywords
Thermal energy storage, design optimization, genetic algorithm, phase change modelling

Klúčové slova
Tepelný výměník, tvarová optimalizace, genetický algoritmus, modelování změny fáze

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I declare that my thesis entitled is entirely the result of my own work. I have faithfully and accurately cited all my sources, including books, journals, handouts as well as any other media.

Juraj Hliník

I would like to express my sincere gratitude to my supervisor Ing. Lubomír Klimeš, Ph.D. for the useful comments, precious remarks and engagement through the learning process of this master thesis.

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1. Introduction

The energy consumption is a long term worldwide problem. This problem is closely related with an ambition to reduce the greenhouse gases which implies the climate change. Therefore, the usage of renewable sources of energy is a methodology to minimize the harmful impact of the fossil fuels on the environment. One possible way is the usage of a solar thermal systems that have many applications in engineering. From the all various possibilities the solar air system with a thermal energy storage using the phase change material is considered in this thesis.

The second chapter of this thesis deals with a general introduction into thermodynamics and heat transfer. It contains the basic concepts necessary for a full understanding of the next chapters of this thesis. Chapter 3 contains a deeper investigation of the two heat transfer modes – the conduction and convection. Moreover, different initial and boundary conditions are summed up at the end of this chapter.

The following chapter introduces the thermal energy system. The fundamental principles of a solar thermal collector are described also with various possibilities to store the thermal energy. One option is the usage of a thermal energy storage with a phase change material whose concept is crucial for this thesis. Chapter 5 contains two methodologies that can be used for a mathematical modelling of a phase change material. One of them, the specific heat method, is used for a numerical model.

In Chapter 6 an energy balance is explained. It is an appropriate numerical method capable to handle the heat transfer problem. The derivation of the formulas necessary for the correct method implementation is described in this chapter as well. The next chapter discusses the optimization. After a general introduction, the rest of the chapter is aimed to a genetic algorithm.

At the beginning of the practical part which starts with Chapter 8 the model of a thermal energy storage unit is introduced. The appropriate assumptions for a numerical model with some additional information are presented at the end of this chapter.

Chapter 9 deals with results of a design optimization of a thermal energy storage unit. This chapter contains two practical problems which are solved by a genetic algorithm. The obtained results are presented and discussed at the end.

2. Basics to thermodynamics and heat transfer

The goal of this section is to introduce some basic concepts of thermodynamics and heat transfer. These concepts have a significant meaning for engineering problems and occur in many chapters of this thesis. Some terms are just briefly mentioned and are discussed more in the next chapters.

2.1. Thermodynamic system

Thermodynamics is a scientific discipline dealing with the heat and relations to other forms of energy. One of the first steps during the analysis of a thermodynamics problem is to define some certain space domain or a mass quantity on which the next analysis is done. This specified region or a certain quantity of some matter of space that is thermodynamically studied is called *thermodynamic system* or just a system. The system is surrounded by *environment* also called *surroundings* and the boundary between them is called *system boundary* [1].

The systems can be classified as open, closed or isolated based on the exchange of mass or energy between the system and the environment. In an *open system* energy, as well as, mass can be exchanged through the boundary. As the *closed systems* are considered systems where the transfer of energy across the boundaries is allowed but the mass exchange can not occur. Neither the energy nor the matter can be transferred trough the boundary of the system in the *isolated systems*. In this case any interaction is not possible between the system and the surroundings. In the real word a perfect thermal insulation does not exist but it is a good approximation in some cases [1].

The systems can be also classified as control mass or control volume. A system is called a *control mass* when the mass exchange through the boundaries is not allowed. It implies that it is also a closed system. In the case of a *control volume* both the energy and the mass can be exchanged across the boundary and thus it is an open system. Furthermore, the control volume unlike the open system has fixed boundaries or fixed volume [1].

2.2. Energy

Another main concept that was already mentioned is called the *energy*. It is an ability of a system to do work and the unit in SI is joule. There are different forms of energy such as kinetic, potential, thermal, internal, chemical and many others. All forms of energies together are noted as the *total energy* E^{tot}. For the next steps it is appropriate not to only refer to the total amount of energy E^{tot} but to divide it into mechanical energy and internal energy U. *Mechanical energy* obtains kinetic and potential energies, therefore, the internal energy consists of energies such as thermal, chemical, nuclear and others [2].

The term *internal energy* U can be understood as the sum of all forms of energies associated with molecular structure of a system. The amount of internal energy affects intermolecular forces – with adding adequate amount of internal energy to the molecules, their bonds disrupt which affects that the material changes its state. This process is also

well-known as a *phase change*. The opposite phase change process occurs when a sufficient amount of internal energy is taken away from the system [3].

The internal energy related to the phase change is called *latent heat*. The kinetic energy of the molecules[1] belongs also into the internal energy and is closely associated with the temperature. When the temperature of the molecules raises, kinetic energy increases proportionally, as well as, the internal energy. The internal energy related to the kinetic energy is called *sensible heat*. The sensible and latent heat are together called *thermal energy* [3].

2.3. Specific heat

The *specific heat* is a material property defined as the amount of energy necessary to raise the temperature by one Kelvin per unit mass. From its definition it is noticeable that the SI unit for specific heat is J kg^{-1} K^{-1}. However, an identical unit kg^{-1} $°C^{-1}$ is often used. By the specific heat at a constant volume denoted by c_v, it is understood special kind of specific heat that occurs when the volume of mass stays constant. Similarly, the specific heat at constant pressure is denoted by c_p [3].

The incompressible substances are substances those volume do not change when the temperature or the pressure is changed. Moreover, the specific heats for these substances equal to each other $c_p = c_v$ [2]. In those cases is the specific heat denoted by c without a subscript. Commonly solids and liquids are taken as incompressible substances, even though their volumes change. However, this change is regularly negligible [3].

The specific heat depends mainly on the nature of the material, its temperature, pressure and significantly on they way of the process execution [4]. For the incompressible substances it is even more simple, hence the specific heat depends only on the temperature. Also for the ideal gases[2] the specific heat is dependent only on the temperature[3].

One of the most fundamental equations of thermodynamics expresses the change of the internal energy U. This equation is for an incompressible substance ($c_p = c_v = c$) given by [3]

$$\Delta U = mc\Delta T, \tag{2.1}$$

where m is the mass of the system, ΔT is the temperature interval and c is the specific heat. The product of mass and specific heat is called heat capacity.

For an ideal gas where an equality between two mentioned specific heats does not hold in general ($c_p \neq c_v$), the change in the internal energy equals

$$\Delta U = mc_v\Delta T. \tag{2.2}$$

The change of so-called enthalpy H can be obtained by replacing c_v with specific heat at constant pressure c_p

$$\Delta H = mc_p\Delta T. \tag{2.3}$$

[1] Kinetic energy of the molecules relates with translational or rotational motion of the atoms and their vibrations movement

[2] Theoretical concept that obeys the ideal gas law, consisting of particles with null volume with random motion and only elastic collisions

[3] Should not be confused with the perfect gas that is more theoretical concept of the ideal gas with constant specific heat

An enthalpy equals to the sum of the internal energy and the product of pressure and volume $H = U + pV$, where the second term is also called flow energy [3].

Some properties of the system like enthalpy or internal energy depend on the quantity of the matter in the system. Often it is useful to express them per unit mass and denote them by a lower-case letter

$$\Delta u = c_v \Delta T \qquad \Delta h = c_p \Delta T. \tag{2.4}$$

2.4. Heat transfer

Heat is an energy form that can be transferred due to the temperature difference. The transport of thermal energy due to the spatial temperature difference is called heat transfer. Despite thermodynamics and the heat transfer look like very familiar disciplines, there is a crucial basic difference between them – whereas the thermodynamics deals with the heat transferred, the heat transfer provides information on how the heat is transferred and the rates of these transfers [3].

Whenever a spatial temperature difference exists between two systems or within a system, these systems (or system) are not in a thermal equilibrium. That means the heat transfer must occur. There are three different processes of a heat transfer called modes. These modes are conduction, convection and thermal radiation. Two of them are discussed in detail in the following chapter [5].

It is common to refer to the sensible and latent heat as the heat and to their transfer as the heat transfer. This convection is kept for the rest of this thesis. The total amount of transferred heat Q during a time interval Δt can be expressed as

$$Q = \int_t^{t+\Delta t} \dot{Q} \, \mathrm{dt}, \tag{2.5}$$

where $\dot{Q}$ (W) is the heat transfer rate.

The heat transfer is a vector quantity, therefore, the perpendicular area A to the heat transfer direction can be considered. Another useful quantity called heat flux $\dot{Q}''$ can be obtained by the expression

$$\dot{Q}'' = \frac{\dot{Q}}{A}. \tag{2.6}$$

For a more precise analysis of the heat transfer is meaningful to define the steady and the transient states. The heat transfer is called steady, when the temperature at any point is not changing with time, so the medium is in an equilibrium. The heat transfer is transient or unsteady, when the temperature at a given point is changing with time. Furthermore, the heat transfer system is called lumped, when the temperature varies with time but not with the position [3].

2.5. First law of thermodynamics

The law of conservation of energy, also known as the first law of thermodynamics, is one of the most fundamental laws in thermodynamics. It states that the total amount of energy in a system can increase or decrease only by the energy transfer through the

boundaries. If no energy is transferred across the boundaries the total amount of energy keeps unchanged. Despite that, the energy is able to change forms within the system [3].

The ways of energy transfer across the boundary depends on a thermodynamic system. In a case of a closed system, the energy can be transferred by heat transfer and work. In an open system it is done by the heat transfer, the work and the mass flow. During the last mentioned process – mass flow – the energy is also transferred, hence the mass carries energy and this process is called the energy advection. The law of conservation of energy is for both mentioned thermodynamic systems stated in the next definition [2].

Definition 2.5.1. *The increase in the (total) amount of energy stored E_{st}^{tot} in a closed system must equal the amount of energy E_{in}^{tot} that enters the closed system, minus the amount of energy E_{out}^{tot} that leaves the closed system [2]*

$$E_{st}^{tot} = E_{in}^{tot} - E_{out}^{tot}. \tag{2.7}$$

In the rate form it is expressed as

$$\frac{dE_{st}^{tot}}{dt} = \dot{E}_{st} = \dot{E}_{in}^{tot} - \dot{E}_{out}^{tot}. \tag{2.8}$$

A steady-state condition occurs when the inflow and the outflow of the energy are equal, therefore, the amount of the total energy remains constant in the system. So, from the first equation a simplified expression can be obtained

$$E_{in}^{tot} = E_{out}^{tot}. \tag{2.9}$$

2.5.1. Energy conservation for closed systems

Consider a closed system. Furthermore, assume that the system has a null change of the kinetic and the potential energy or equivalently the change in the mechanical energy is zero.

Whereas the total energy consists of the mechanical energy and the internal energy and no change in the mechanical energy occurs for the system, only the amount of the internal energy can be changed. In this case the next equation holds

$$E_{in}^{tot} - E_{out}^{tot} = \Delta U = mc_v\Delta T. \tag{2.10}$$

The specific heat at a constant volume c_v can by replaced by the specific heat c for the incompressible substances. Furthermore, without the work done by the system with only the heat transfer trough boundaries, the amount of heat Q transferred through the boundaries can be expressed as

$$Q = mc_v\Delta T. \tag{2.11}$$

2.5.2. Energy conservation for steady-state uniform flow systems

When a studied problem contains the fluid flow, the system is modelled as a control volume. The uniform flow means there are the same property values in a whole system at any instant of the time. In addition, consider a steady-state flow through a pipe or a duct. In that case the fluid flow can be after suitable analysis considered as one-dimensional which leads to a significant simplification.

To study the conservation of the energy for the fluid flows, the mass flow rate $\dot{m}$ (kg s^{-1}) has to be introduced. The mass flow rate expresses the amount of the fluid mass passing a plane A_c per unit time. The plane A_c is a cross-sectional with respect to the direction of the fluid flow. For the fluid flow with velocity v and density ρ and with respect to all mentioned conditions the mass flow rate equals [3]

$$\dot{m} = \rho v A_c. \tag{2.12}$$

Related and also often used volumetric flow rate $\dot{V}$ can be obtained as

$$\dot{V} = v A_c \qquad or \qquad \dot{V}\rho = \dot{m}. \tag{2.13}$$

Furthermore, the conservation of mass guarantees that mass flow rate remains constant, even for tubes with changing diameter. For the system without work and negligible change in the mechanical energy the first law of thermodynamics in rate form looks like

$$\dot{Q} = \dot{m}\Delta h = \dot{m} c_p \Delta T \tag{2.14}$$

2.5.3. Energy conservation for the surface

The special case of the conservation of energy is applied for the surface of a medium. A surface can not store or generate any energy, since the surface is volumeless. Therefore, what enters from one side has to leave from another [2]

$$\dot{E}_{in} = \dot{E}_{out}. \tag{2.15}$$

Classical example of the surface energy balance is shown in Figure 2.1. Three modes of a heat transfer act on the control surface. Conduction $\dot{Q}_1$ occurs from the material to the control surface and the convection $\dot{Q}_2$ with radiation $\dot{Q}_3$ from the control surface to the outflow fluid

$$\dot{Q}_1 = \dot{Q}_2 + \dot{Q}_3. \tag{2.16}$$

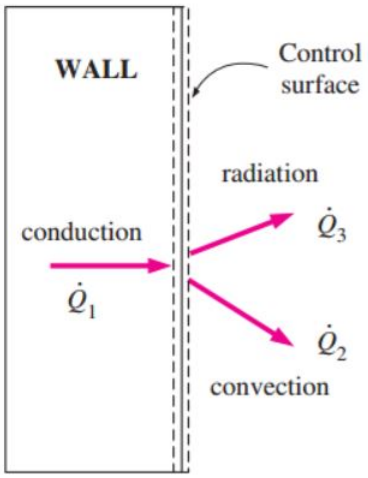

Figure 2.1: Energy conservation on the surface [3]

2.5.4. Thermal and mechanical energy equation

Mechanical and thermal energies lead to important statement that is useful for the heat transfer analysis. It is appropriate to have in the mind that even though the total amount of energy is conserved, the energy can still change forms.

One important process for later heat transfer analysis is called heat generation. It occurs when some kind of internal energy is conversed into thermal energy [2]. The heat generation per unit volume, whose SI unit is W m^{-3}, is often denoted by $\dot{g}$. The heat generation in some general volume V equals to

$$\dot{G} = \int_V \dot{g} \, \mathrm{dV}, \tag{2.17}$$

that is simplified to $\dot{G} = \dot{g}V$ for homogeneous material[4] [3].

Using the first law of thermodynamics, the next statement useful for heat transfer analysis can be achieved.

Definition 2.5.2 (Thermal and mechanical energy equation at an instant time)**.** *The rate of increase of thermal and mechanical energy $\dot{E}_{st}$ stored in the control volume must equal the rate at which thermal and mechanical energy $\dot{E}_{in}$ enters the control volume, minus the rate at which thermal and mechanical $\dot{E}_{out}$ energy leaves the control volume, plus the rate at which thermal and mechanical energy $\dot{E}_g$ is generated within the control volume [2].*

$$\dot{E}_{st} \equiv= \frac{dE_{st}}{dt} = \dot{E}_{in} - \dot{E}_{out} + \dot{E}_g \tag{2.18}$$

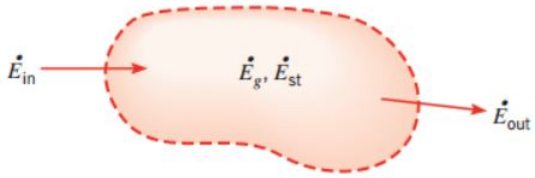

Figure 2.2: Thermal and mechanical energy conservation at an instant time [2]

[4] a homogeneous material has the same property value at any point

3. Heat transfer modes

The heat transfer can not be neglected and has to be considered in many application where appropriate geometry, thickness or optimal material affect an efficiency and the practical use. As was already mentioned, the heat transfer can be done by three modes - conduction, convection and radiation. To do a deeper heat transfer analysis it is necessary to discuss them separately.

All three modes often occur simultaneously in real situations. However, familiarity with the first two mentioned modes is sufficient for this thesis. The radiation is well-discussed in both main sources for this chapter which are [2] and [3].

3.1. Conduction

It is a kind of a heat transfer that develops across the medium. The medium can be solid or a stationary fluid. On a microscopic scale the conduction can be seen as energy transfer between the interacting particles with different amount of energy. By the second law of thermodynamics the transfer of energy always occurs from more energetic particles to the less energetic one caused by microscopic collisions. This heat transfer would work even without collisions, but they enhance the energy transfer. The conduction appears in gases, liquids or solids and the concept is quite similar in these states, just the fluids unlike the gases have stronger and more frequent interactions due to the higher molecular densities. The conduction has the most significant meaning in the solid where the heat transfer is based on the lattice vibrations and the free electrons movement [2].

3.1.1. Fourier's law

If the heat transfer is dependent on the time and is significant in all three spatial coordinates, the general form of the heat conduction can be achieved. The heat flow direction is perpendicular to the constant temperature surface and is oriented in the decreasing temperature direction. The conduction rate equation can be expressed by the equation known as Fourier's law that can be expressed [3]

$$\dot{Q} = -kA\nabla T \tag{3.1}$$

or similarly the heat flux can be obtained by

$$Q'' = -k\nabla T \tag{3.2}$$

where k (W m^{-1} K^{-1}) is the thermal conductivity, A (m^2) is the cross-sectional area and ∇T represents the temperature gradient. The minus sign can be described by fact that the heat transfer must occur in the direction of decreasing temperature.

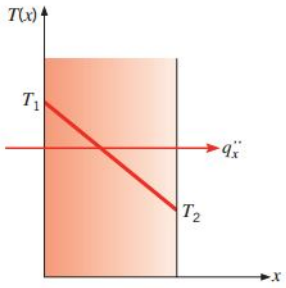

Figure 3.1: Heat transfer by conduction in 1D [2]

3.1.2. Properties

The knowledge about the material and its material properties is important for the heat study transfer analysis. The simplification for a practical use can be obtained if the material property has the same value in all space coordinates or at least the change is negligible. These materials are also well-known as isotropic materials.

The category of properties meaningful for the heat transfer are called thermophysical. It can be furthermore divided into two distinct subcategories – transport and thermodynamic properties. The transport properties are harder to measure and include a coefficient of diffusion rate. For example the thermal conductivity k for diffusion rate of heat, kinematic viscosity μ for the diffusion of momentum or coefficients of another diffusions such as diffusion of composition or electrical conductivity [2].

The most important transport property for the heat transfer is the thermal conductivity that is used in Fourier's law. It is crucial material property that can be interpreted as the material ability to conduct the heat. Mainly in anisotropic materials like wood or laminated composite materials this property value varies depending on the space coordinates and is represented by a tensor in the three dimensional case. It is the macroscopic representation of a molecular contribution to the heat conduction, that is closely related with the state of a given material [6]. For the majority of substances the thermal conductivity is dependent on the temperature, however, in many computations changes of thermal conductivity are negligible for a given temperature interval. The kinetic theory for gases can be used to evaluate analytically the thermal conductivity, however, in general it is usually experimentally measured. The material can be used as a good heat conductor if the thermal conductivity reaches high values and it can be used as the insulator otherwise [3].

However, even though the thermal conductivity has a significant meaning for the heat transfer analysis, the category of the thermodynamic properties is more crucial. That is the category referred to the equilibrium state of the material [2]. Very commonly used properties from this category are the density ρ and the specific heat c that were already mentioned in the first chapter.

Another useful material property for the heat transfer analysis is thermal diffusivity that can be composed from another three properties as follows

$$\alpha = \frac{k}{\rho c_p}, \tag{3.3}$$

where $c_p = c$ for incompressible substances.

The product in a denominator is called volumetric heat capacity of a material. Therefore, the thermal diffusivity represents the ratio between the conducted heat and the heat stored per unit volume. In other words it expresses how fast the heat transfers in a material.

Thermal resistance is another important material property for the heat transfer analysis. Even though the thermal resistance can be used for solving a complicated problem containing multilayer plane walls with different properties for each layer, a more simpler concept is sufficient for this thesis.

The thermal resistance R for the conduction is called the conduction resistance and for a wall of thickness L and with cross-sectional area A with respect to the heat transfer direction equal [2]

$$R = \frac{L}{kA} \tag{3.4}$$

3.1.3. Fourier-Biot equation

The goal of this section is to express the Fourier-Biot equation using the energy balance. Consider the most general case, when the heat conduction is significant in all three spatial dimensions. The heat transfer is moreover transient and even the heat generation is included. Also consider a control volume element which dimensions are $\Delta x, \Delta y, \Delta z$ as in Figure 3.2. Hence it is possible to express the volume of the element as $V_{control} = \Delta x \Delta y \Delta z$ and $\dot{G}_{control} = \dot{g} V_{control} = \dot{g} \Delta x \Delta y \Delta z$. Applying the energy balance during time interval Δt, following equation can be obtained [3]

$$\dot{Q}_x + \dot{Q}_y + \dot{Q}_z - \dot{Q}_{x+\Delta x} - \dot{Q}_{y+\Delta y} - \dot{Q}_{z+\Delta z} + \dot{g} \Delta x \Delta y \Delta z = \frac{\Delta E_{control}}{\Delta t}. \tag{3.5}$$

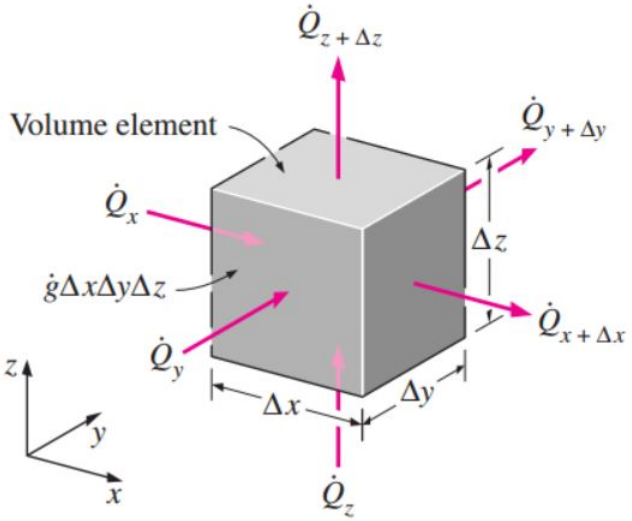

Figure 3.2: Energy balance for control volume element [3]

The term on the right side expresses the rate of the energy content change of a given element. No work is done in the element and the volume element that is either solid or liquid can be considered as an incompressible substance. In other words it can be replaced by

$$\Delta E_{control} = mc(T^{t+\Delta t} - T^t) = c\rho \Delta x \Delta y \Delta z (T^{t+\Delta t} - T^t). \tag{3.6}$$

Substituting $\Delta E_{control}$ and dividing by $V_{control}$ Equation (3.5) changes into

$$-\frac{1}{\Delta y\Delta z}\frac{\dot{Q}_{x+\Delta x}-\dot{Q}_x}{\Delta x}-\frac{1}{\Delta x\Delta z}\frac{\dot{Q}_{y+\Delta y}-\dot{Q}_y}{\Delta y}- \\ -\frac{1}{\Delta x\Delta y}\frac{\dot{Q}_{z+\Delta z}-\dot{Q}_z}{\Delta z}+\dot{g}=c\rho\frac{(T^{t+\Delta t}-T^t)}{\Delta t} \tag{3.7}$$

The first term in the previous equation in case of limit $\Delta x \to 0$ and with using Fourier's law gives

$$\lim_{\Delta x\to 0}\left(-\frac{1}{\Delta y\Delta z}\frac{\dot{Q}_{x+\Delta x}-\dot{Q}_x}{\Delta x}\right)=-\frac{1}{\Delta y\Delta z}\frac{\partial \dot{Q}_x}{\partial x}= \\ =-\frac{1}{\Delta y\Delta z}\frac{\partial}{\partial x}\left(-k\Delta y\Delta z\frac{\partial T}{\partial x}\right)=\frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right) \tag{3.8}$$

Similarly taking limit for another two dimensions and for the time increment Equation (3.7) can be expressed as

$$\frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(k\frac{\partial T}{\partial y}\right)+\frac{\partial}{\partial z}\left(k\frac{\partial T}{\partial z}\right)+\dot{g}=c\rho\frac{\partial T}{\partial t} \tag{3.9}$$

or for the constant thermal conductivity k

$$\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}+\frac{\partial^2 T}{\partial z^2}+\frac{\dot{g}}{k}=\frac{1}{\alpha}\frac{\partial T}{\partial t} \tag{3.10}$$

where α is the thermal diffusivity described above in this chapter. This last equation is called the Fourier-Biot equation [3]. Also some others important well-known forms of this equation can be obtained under some considerations. In the case of steady heat transfer Poisson equation is obtained

$$\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}+\frac{\partial^2 T}{\partial z^2}+\frac{\dot{g}}{k}=0 \tag{3.11}$$

For transient heat transfer without generation obtained equation is called diffusion equation

$$\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}+\frac{\partial^2 T}{\partial z^2}=\frac{1}{\alpha}\frac{\partial T}{\partial t} \tag{3.12}$$

It is called Laplace equation if it is steady heat transfer without heat generation

$$\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}+\frac{\partial^2 T}{\partial z^2}=0 \tag{3.13}$$

Another and more deeper equation derivation can be found in [7].

3.2. Convection

The convection is the heat transfer mode for which an existence of a solid surface and adjacent moving fluid with temperature gradient between them is necessary. The convection is a transfer of energy caused by random molecular motion (conduction) and by the

bulk motion of the fluid [3]. The presence of a bulk motion of the fluid improves the heat exchange in comparison to the conduction. The heat transfer by convection can occur in liquids and gases but not in solids due to their relatively fixed molecules. The process, in which the energy is transported just by the bulk motion is called advection [2]. The higher speed of the fluid motion provides the better convection.

The sensible and also the latent heat can be transferred by a convection. The first one mentioned is more typical but there are also examples of the latent heat exchange in case of a phase change of the fluid [2]. A good example is the boiling, when the boiling fluid generates raising vapour bubbles. These bubbles then indicate the heat transfer by convection.

Two types of the convection are distinguished – when there is an external generator of the fluid flow and when there is not. A forced convection means the presence of an external source of the flow, such as a pump or a fan. A free (or natural) convection occurs when the flow is caused due to the density gradients in fluids with action of the gravitational force. Sometimes both types of convection are present and then we refer to them as mixed convection [2].

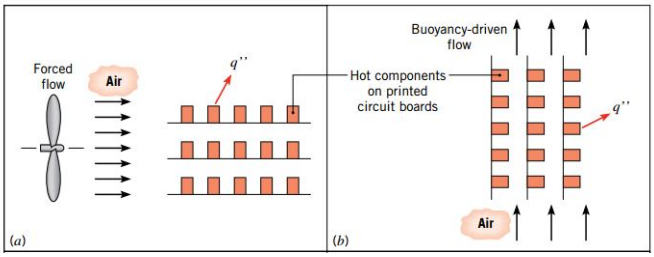

Figure 3.3: Forced and natural convection [2]

3.2.1. Newton's law of cooling

The convection is a very complex mode of the heat transfer and closely depends on the fluid properties and also on the geometry of the solid surface and its roughness. Some of these fluid properties are dynamic viscosity μ , velocity, density and the type of fluid flow (see section 3.2.3). Even though it looks like a complex problem the rate of heat transferred by the convection can be easily expressed by Newton's law of cooling in form [2]

$$\dot{Q} = hA(T_s - T_\infty) \tag{3.14}$$

or in the case of the heat flux

$$\dot{Q}'' = h(T_s - T_\infty), \tag{3.15}$$

where A is the surface area of the heat transfer, h (W m^{-2} K^{-1}) is the convective heat transfer coefficient and the parentheses contain the difference between the temperature of the surface T_s and the ambient fluid temperature T_∞. The convective heat transfer coefficient h depends also on the properties mentioned in the first paragraph of this section and it is a complex task to determine it.

3.2.2. Velocity and temperature boundary layers

The term T_∞ used in Newton's law of cooling is more precisely a fluid temperature at sufficient distance from the surface. The goal of this section is to make a better understanding in a 'sufficient distance'.

Consider the cooling of a heated surface by a fluid flowing over this surface as in Figure 3.4. As can be seen, the velocity of the fluid and the temperature vary in the vicinity of the surface. At the interface of the fluid and impermeable[1] surface fluid velocity has zero magnitude. This condition is called no-slip condition and it is related with the fluid viscosity [3]. This condition forms the velocity profile – consider the fluid flow as the layers stored at each other. The most bottom layer with a zero velocity slows down the upper layer because of the shear stresses[2] acting between them [2]. This process continues up to a distance $y = \delta$ in the normal direction from the surface, where this friction becomes negligible. With the increasing distance from the surface velocity profile tends to finite value u_∞ – velocity of the outer flow (not influenced by close presence of the heated surface). A value δ is mostly obtained as a distance y in the normal direction from surface for which is $u = 0,99u_\infty$ valid. The region from the surface up to δ, where the effects of shear stresses are significant is termed as the velocity boundary layer and δ is called velocity boundary layer thickness. The zone above the boundary layer is called inviscid flow region. On Figure 3.4 can be seen that the velocity boundary layer thickness (dashed line) is increasing from the leading edge in the direction of the fluid flow [2] [3].

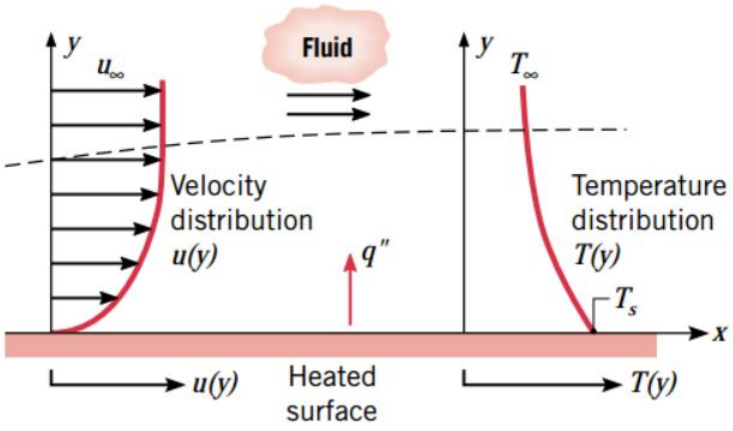

Figure 3.4: Boundary layers [2]

Considering again the same example of cooling the heated surface with the fluid that has the ambient temperature T_∞. Whereas $T_s > T_\infty$ convection occurs from the heated surface to the fluid and because of the continuity of the temperature, the fluid particles adjacent to the surface achieve temperature T_s. With a similarity to the velocity boundary layer, the temperature varies in the region called thermal boundary layer and its size in general differs from the size of the velocity boundary layer. The thickness of the temperature boundary layer δ_t is mostly defined as a distance y for which $(T_s - T)/(T_s - T_\infty) = 0.99$ is valid [2]. In the region, where the velocity of the fluid is low, the heat transfer by a random molecular motion of the fluid is significant (at the interface between these two mediums, it is the only mechanism of the heat transfer) [2].

[1] a solid the surface through that fluid can not penetrate
[2] it is caused by the force vector component parallel to the fluid velocity

3.2.3. Fluid flow classification

The analysis of the fluid flow leads to the study of the convection, what is a valid reason to classify the flows into groups for their easier study. Some of the most important and general classifications are going to be discussed below. All these types of classifications are discussed in [3].

One of the most important classifications is based on the compressibility of the fluid. In this case the fluid flow is divided into compressible or incompressible based on the density variation. The density variation is commonly irrelevant for the liquids and they are generally taken as incompressible, on the other hand, the gases are compressible .

Flow is said to be internal if the fluid flows through the channel and the channel is completely filled with this fluid. If the channel is not completely filled with the fluid it is called open-channel flow. An external flow is the case when the fluid flows over a surface. Based on the time dependence similarly like in the conduction we can split the fluid flows to steady and transient. Another classification that was already mentioned above splits the flows into forced or natural depending on the presence of external flow generator.

An extremely significant meaning for the fluid flow study has a classification into laminar or turbulent flow. Huge importance has also a dimensionless quantity that predicts these kinds of the fluid flow and they are discussed together in the next section.

3.2.4. Laminar and turbulent flow

The laminar flow occurs when the fluid particles movement is highly ordered and predictable in smooth streamlines[3]. The turbulent flow in the contrary is an irregular, disordered motion of the fluid particles at higher velocities [2]. Also there is a form of a flow that contains a mixture of laminar and turbulent flow called transitional flow. A difference of how laminar or turbulent flow can look is shown in Figure 3.5

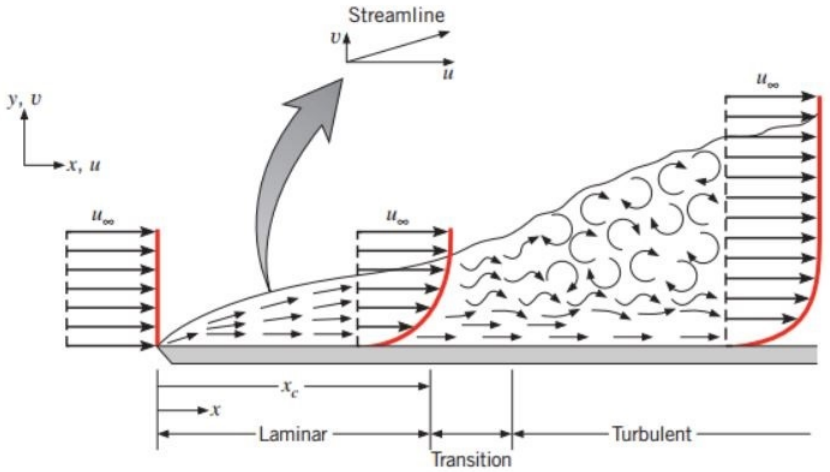

Figure 3.5: Velocity boundary layer and difference between laminar and turbulent flow [2]

The question that has to be in many cases answered in a convection heat transfer problems is if a fluid flow in the boundary layer is laminar or turbulent. A velocity

[3]imaginary curves parallel to the velocity vector at all points

boundary layer can contain laminar, as well as, turbulent flow with a zone of turbulent flow where the laminar flow changes to turbulent. In a turbulent layer, the vortices are developed quite close to the surface. They can move in waves with nonlinear interaction that has impact on the irregular behaviour and causes growth of the turbulent layer thickness [2]. It also increases the heat transfer and the heat transfer coefficient achieves the highest values at this zone.

Reynolds number [3]

The specifications if the fluid flow is laminar or turbulent depends on many parameters. Instinctively the surface properties as the temperature, the geometry and also the roughness have crucial influence, as well as, the fluid flow types as those mentioned above in a Section 3.2.3. However the main aspects on which the fluid flow depends were observed by O. Reynolds after whom this quantity is called Reynolds number. Reynolds number is dimensionless and is defined as follows

$$Re = \frac{vL_c}{\nu}, \tag{3.16}$$

where u (m s^{-1}) is the velocity, L_c (m) is a characteristic length associated with a geometry and ν (m^2 s) is the kinematic viscosity.

Higher values of Reynolds numbers express that the inertia forces are dominant in comparison with the viscous forces. So the viscous effect are not able to avoid the turbulent intense mixing effects and therefore the higher values of Reynolds number represent the turbulent flow. On the other hand, for smaller values of Reynolds number viscous forces are significant and it implies that the flow is laminar. The value of the Reynolds number at which the flow changes from laminar to turbulent is called critical Reynolds number.

3.2.5. Another important dimensionless quantities

The list of the dimensionless quantities that are used regularly in the heat transfer problems is quite long. Reynolds number is one of them but there are other significant ones. Another one is Nusselt number [3] that expresses the ratio of the convection h and the conduction coefficient k_{fluid} of the fluid as follows

$$Nu = \frac{hL_c}{k_{fluid}} \tag{3.17}$$

where L_c is a characteristic length. Prandtl number [3] is also a dimensionless quantity that is the ratio of the momentum and the thermal diffusivity

$$Pr = \frac{c_p \mu}{k}. \tag{3.18}$$

It expresses the relation between the thermal and the velocity boundary layer thickness. For $Pr \ll 1$ the heat diffusion is much more significant then the momentum diffusivity and also the thermal boundary layer is thicker than the velocity boundary layer.

Fourier number Fo [3] expresses the rate between the heat conducted through the volume and the stored heat. Larger values determine the faster heat transport through a material.

$$Fo = \frac{\alpha t}{L_c^2} = \frac{k_{fluid}}{\rho c} \frac{t}{L_c^2}. \tag{3.19}$$

A last quantity mentioned is Biot number Bi [3]

$$Bi = \frac{hL_c}{k_{solid}} \tag{3.20}$$

It should be noted that Biot number differs from Nusselt number in the denominator. Biot number expresses the ratio between the conduction resistance inside of the solid material R_{cond} and the convection resistance at the surface R_{conv}

$$R_{cond} = \frac{L}{k_{solid}A} \qquad R_{conv} = \frac{1}{hA}. \tag{3.21}$$

For $Bi \ll 1$ conduction is much faster and significant than convection at the surface.

3.2.6. Internal flow

The heat transfer systems consists of many pipes or ducts trough which the fluid transfers. Consequently, the focus should be aimed for deeper understanding of an internal flow. Furthermore, in general the fluid transport is guaranteed by the pump and therefore it can be categorized also as a forced convection problem.

The study of the internal flows contains enormous amount of quantities or different problems based on the material geometry, the fluid flow or the surface conditions. However, a fully theoretical understanding with the analytic solutions have only some of the most basic cases. For the rest are the experimental results given that may sometimes lead to the notable errors. This chapter will contain only those quantities and studied problems which are important for next chapters of this thesis.

Flow characterization

It was already mentioned that the fluid flowing over some surface develops with the increasing distance from the leading edge. Consider a similar case of a laminar flow entering the circular pipe with a uniform velocity. From a no-slip condition on the pipe walls and due to its symmetric profile, the velocity boundary layer grows symmetrically. The distance from the beginning up to the position when these boundary layers merge at the centreline is called hydrodynamic entry length $x_{fd,h}$ [3]. The region beyond this value is called hydrodynamically fully developed region. Up to $x_{fd,h}$ the velocity profile develops and from this point the velocity profile keeps an unchanged parabolic shape.

Similarly, the concept of the thermal entry length $x_{fd,t}$ and the fully thermal boundary layer can be done. Furthermore, a important result for a fully thermal boundary layer is that the convection coefficient stays constant for a fully thermal boundary layer [3].

A parabolic shape of a velocity profile is very inconvenient for the calculations. It is appropriate to work with the mean velocity u_m that can be for incompressible flow obtained from

$$\dot{m} = \rho u_m A_c. \tag{3.22}$$

This result can be used for the calculations of a Reynolds number

$$Re = \frac{v_m L_c}{\nu} \qquad L_c = \frac{4A_c}{P} \tag{3.23}$$

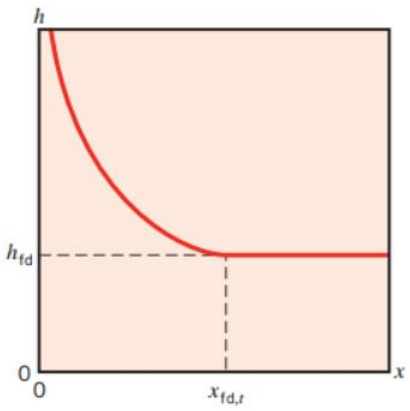

Figure 3.6: Variation of the convection heat transfer coefficient for pipe [2]

where L_c is the characteristic length of a given pipe/duct and A_c is its cross-sectional area and P is its perimeter.

In general the flow in tubes can be considered as a laminar flow for $Re \leq 2300$ and turbulent flow for $Re \geq 10000$. The transitional flow is considered between these two numbers.

Determination of a Nusselt number

The knowledge of a convection coefficient is crucial for a flow study, practically, the convection coefficient is obtained from the Nusselt number. There is a really limited number of cases when the Nusselt number is not represented by an empirical correlation [2]. It should be noted that the most fitting correlation with respect to a given propositions does not have to represent a real-life situation.

For a laminar fully developed flow the Nusselt number remains constant and therefore is easier to estimate. Higher heat transfer coefficients are obtained for turbulent flow, which is often the reason for turbulent flow utilization. However, the Nusselt number is determined from empirical correlations.

3.3. Boundary and initial conditions

To obtain a particular solution of some heat transfer equation it is necessary to specify the boundary and in the case of time dependence also an initial condition.

The first kind of the boundary condition is a constant temperature on the surface also called Dirichlet condition. As an example in one dimension, the boundary conditions for the plane wall of thickness L can look as [3]

$$T(0,t) = T_0 \qquad T(L,t) = T_L. \tag{3.24}$$

Another type of a boundary condition is the specified heat flux at the surface. When the heat flux is constant or fixed it is called Neumann condition or the second kind of a boundary condition and from Fourier's law [3]

$$\dot{Q}''_x(0) = -k\frac{\partial T(0,t)}{\partial x} \qquad \dot{Q}''_x(L) = -k\frac{\partial T(L,t)}{\partial x}. \tag{3.25}$$

The values of $\dot{Q}''_x(0)$ or $\dot{Q}''_x(L)$ equal to zero when the surface is insulated.

The presence of a moving fluid is used also for the boundary condition of the third kind that is shown in Figure 3.7. It is a typical boundary condition for many engineering heat transfer problems. Another common used name is the convection surface condition and is obtained from the surface energy balance [3].

$$-k\frac{\partial T(0,t)}{\partial x} = h[T_\infty - T(0,t)] = \dot{Q}''_{conv} \tag{3.26}$$

The term $\dot{Q}''_{conv}$ is convective heat flux that is going to be explained in next section.

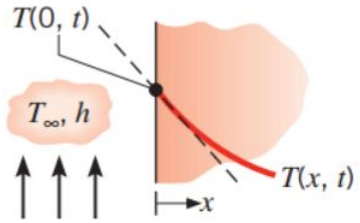

Figure 3.7: Convection surface condition [2]

4. Thermal energy storage

For many years the topic of renewable sources of energy is well-discussed via all forms of media. A worldwide ambition is to reduce the greenhouse gases which implies the climate change. Therefore, the usage of renewable energy sources increases with respect to the minimization of the environmental impact. The solar energy is one possibility with a wide range of applications. The two most progressive fields are the drying of the products and the space heating. Buildings account about 40% of the total primary energy[1] consumption in a European Union [9]. A huge impact on the total amount of energy consumption in buildings has the space heating and air-conditioning [10]. That provides the opportunities for a huge investigation and developments of a better usage of the energy and its conservation.

A solar thermal system[2] is one possibility for the heating or cooling buildings. In general, these systems convert the solar radiation[3] into the thermal energy that is distributed by a moving fluid [11]. The system is called solar air system in the case of the energy transport by air. The main part of these systems are special kinds of heat exchangers called solar collectors which are mounted on the walls or on the roof of the buildings.

4.1. Solar thermal collector

One of the most used types for residential buildings is a flat plate collector with a simple construction and low capital costs [12]. The possible design can be seen in Figure 8.2. The main construction is made by an insulation provided at the back and side walls to minimize the heat losses by conduction. The top of the collector is mostly covered by one or two layers of a transparent glass to reduce an upward convection and to keep the heat inside. This cover is also called glazing. An absorber plate often made of a metal that is a good conductor of the heat that absorbs the solar radiation and changes it into the thermal energy is situated inside the collector. When the temperature of the absorber is higher than the temperature of the moving transport fluid, the natural convection from the absorber into the fluid must occur. A net of tubes or channels with a circulating fluid secures the transport of the thermal energy from a absorber into the building unit [11]. Mainly in commercial applications where the primary goal is the ventilation and the space heating needs are restricted the usage of a solar air collector without glazing is applicable [13].

Water is another commonly used fluid for the thermal energy transfer. The water-based solar collectors transport water through the collector which can in some occasions lead to freezing of the water or its leaking [14]. On the other hand, the convenient properties of the water compensate these disadvantages. Mainly the ability to conduct more heat than air and its higher volumetric heat capacity [15].

Collectors can be split into stationary and concentrating by the ability to track the Sun. For a cheap flat plate collectors with low temperature range (up to 100 °C) it

[1] Primary energy is an energy stored in natural resources before any conversion process [8]

[2] They should not be confused with solar photovoltaic systems, which convert solar radiation into electricity

[3] Hence, this chapter marginally contains term radiation, at least briefly explanation should be used. The process in which an energy is emitted by matter is called radiation. Any matter of non-zero temperature emits an energy [2]

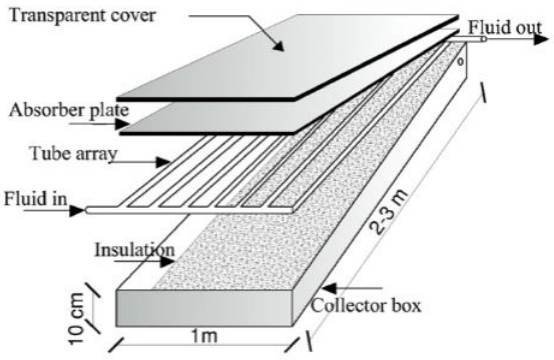

Figure 4.1: Solar air collector [11]

is inconvenient to be concentrating. The typical examples of concentrating collectors are the parabolic shape collectors, which reflect rays from the Sun into a smaller area which increases the radiation flux [11]. Various types of solar thermal collector and their classifications can be found in [11].

When the obtained thermal energy should be stored for the later usage, the solar air systems have to contain some temporary storage called the thermal energy storage. One of the most suitable choices is a choice of a thermal energy storage unit with a phase change material. This next section discuss about these two concepts and the reason why a phase change material is more appropriate for a heat storage.

4.2. Thermal energy storage

The solar energy is intermittent which causes a variation in the energy supply. A convenient solution to reduce a mismatch with the energy demand is a usage of a thermal energy storage. The usage of this storage unit is convenient for wide range of applications [16]. The thermal energy storage should provide a good storage, as well as, an efficient extraction of a stored energy and should be insulated [17].

The stored thermal heat has to be retrieved in a need, therefore, some reversible process has to be chosen to store the heat [18]. Depending on the application a reversible storage of heat can be provided by three basic methods: sensible heat storage, latent heat storage and chemical reactions. However, just the first two mentioned are widely applicable [18]. The latent heat storage uses a phase change to store the energy and from all possible phase change combinations only three are commercially used as can be seen in Figure 4.2. The appropriate choice of a thermal energy storage depends on the storage period and operating conditions which are often space limited [17].

Sensible heat storage

The sensible heat is obtained in a physical process in which the stored heat causes the increase of the temperature in the storage material without change of its phase. The amount of stored heat – sensible heat – can be calculated as [18]

$$\dot{Q} = m \int_{T_1}^{T_2} c_p dT, \tag{4.1}$$

where c_p is the specific heat at constant pressure, m is the mass and T is the temperature. The volumetric heat capacity of gases is very small therefore this method has applications

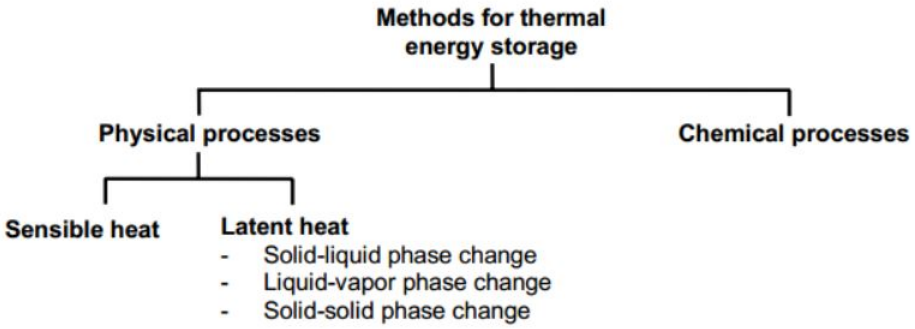

Figure 4.2: Reversible storage methods [18]

mainly for the solids and liquids as the storage material [18]. Contrarily, the sensible heat is released from the material when the fluid flowing in the adjacency of the storage material has the lower temperature.

Latent heat storage

An essential feature of the latent heat storage is the ability to provide a higher energy storage density for a material undergoing the phase change in comparison to many other materials with the sensible heat storage under the same conditions. However, it is possible that the materials without the phase change can even though store more energy, as the result of some materials properties like a volumetric heat capacity [15]. The amount of a stored or released latent heat during the completely finished process of a phase change can be expressed as

$$E_{st} = mL, \tag{4.2}$$

where L (J kg^{-1}) is the specific latent heat.

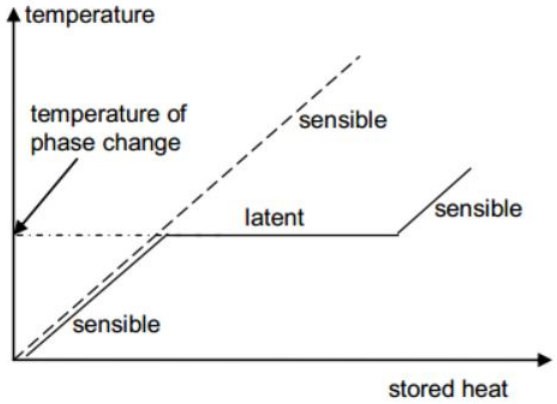

Figure 4.3: Dependence of energy storage on temperature and phase change [18]

The main advantage of a latent heat storage is shown in Figure 8.2. It should be noted that during the phase change the temperature of the material can slightly differ. This property can be used for the stabilization of the temperature in some applications [18].

TES with latent heat storage

When the latent heat storage is considered several aspects are required [19] from a choice of the most suitable material:

1. As a phase change material should be chosen that one whose melting temperature is in the desired temperature range
2. High values of density and latent heat to improve the energy storage
3. Thermal and chemical stability
4. An appropriate volume change during the phase change
5. Small subcooling[4]

An economical aspects as price and availability should be also considered for a proper choice of a material. Full list of other important properties can be found in [19] or [20].

As it was mentioned, not all types of a phase change are appropriate for a thermal energy storage. Even though the solid-liquid phase change has in general high values of latent heat the unacceptable volume expansions limit its possible applications [19].

Phase change materials (PCM) can be at this point further categorized to organic, inorganic and eutectic materials. Paraffin is one of the most common organic PCMs. Paraffin waxes have an average thermal storage density with the reasonable price. They are chemically stable and thermally stable and very small subcooling occurs for the solidification phase change [19]. Their various types guarantee different melting temperatures.

[4]Subcooling refers to effect when during solidification the temperature below melting temperature has to be obtain to begin solidification [18]

5. Phase change modelling

The problem of a solid-liquid phase change can be modelled by a heat transfer equation with a heat generation [21]. For the purposes of this thesis a two dimensional case is considered

$$\rho c_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(k\frac{\partial T}{\partial y}\right) + \dot{Q}, \tag{5.1}$$

where ρ (kg m^{-3}) is the density, c_p (kJ kg^{-1} K^{-1}) represents the specific heat at constant pressure, k (W m^{-1} K^{-1}) is the thermal conductivity, T (K) denotes temperature, $\mathbf{x} = (x, y)$ are the spatial coordinates and $\dot{Q}$ (W m^{-3}) is the internal source of heat.

The term $\dot{Q}$ describes the rate of latent heat evolution during the liquid-solid phase change and can be described as follows [21]

$$\dot{Q} = \rho L_f \frac{\partial f_s\left(\mathbf{x}, t\right)}{\partial t}, \tag{5.2}$$

where L_f (kJ kg^{-1}) represents the specific latent heat of fusion and f_s is the solid phase fraction. Therefore, the solid phase fraction can take values from 0 up to 1 where $f_s = 0$ means that the material is just in the liquid phase and similarly, $f_s = 1$ means that the material is completely in the solid phase [22].

Enthalpy method

For the phase change of the material various approaches are used [21]. One significantly important is the enthalpy method. Even though an enthalpy can depend on more variables, for many models the enthalpy is expressed just as a function of the temperature [23]. For the reference temperature T_{ref} that is below solidus temperature[1] T_s the enthalpy function is defined as [23]

$$H(T) = \begin{cases} \int_{T_{ref}}^{T} c\rho d\theta & \text{for } T < T_s \\ \int_{T_s}^{T} (c\rho - \rho L_f \frac{\partial f_s}{\partial t}) d\theta & \text{for } T_s \leq T \leq T_l \\ \int_{T_l}^{T} c\rho d\theta & \text{for } T > T_l \end{cases} \tag{5.3}$$

where T_l is the liquidus temperature[2]. For a temperature interval between solidus and liquidus temperature during the melting process[3] a solid fraction is a non-increasing function with respect to time whereas its time derivation will be always negative or null.

Two possible curves describing a relation between the enthalpy and the temperature are shown in Figure 5.1. Mainly for the pure metals a typical characterization is that the latent heat is evolved isothermally at a constant melting temperature as can be seen in case (a). For majority of the materials, however, the latent heat of fusion is evolved in the temperature range characterized by a solidus and liquidus temperature. As an example a linear dependence is shown in Figure 5.1 (b) [24].

[1] Temperature, below which is $f_s = 1$
[2] Temperature, above which is $f_s = 0$
[3] Similarly, for the congealing a solid fraction is a non-decreasing function

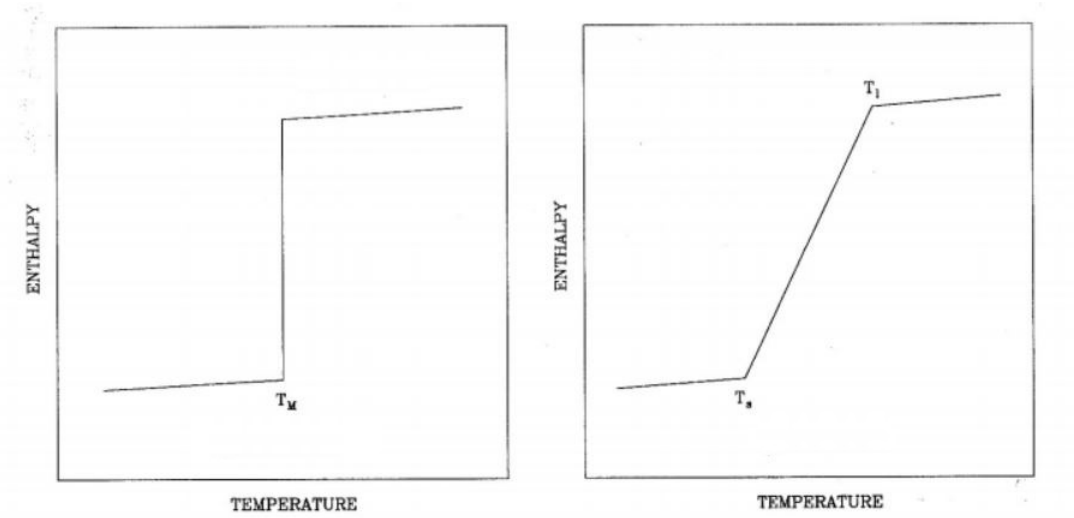

Figure 5.1: Evolution of the latent heat evolution (a) isothermal (b)linear [24]

Specific heat method

The purpose of this method is a usage of so-called the effective specific heat c_{eff} to comprise the latent heat. It can be derived from previous method and is defined as [21]

$$c_{eff}\,(T) = \frac{1}{\rho}\frac{\partial H}{\partial T} \tag{5.4}$$

Therefore the effective specific heat can be expressed as

$$c_{eff(T)} = \begin{cases} c & \text{for } T < T_s \\ c - L_f \frac{\partial f_s}{\partial t} & \text{for } T_s \leq T \leq T_l \\ c & \text{for } T > T_l \end{cases} \tag{5.5}$$

By substituting obtained effective specific heat c_{eff} into Equation (5.1) the following result can be obtained

$$\rho c_{eff}\frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(k\frac{\partial T}{\partial y}\right) \tag{5.6}$$

When a material is not undergoing a phase change the effective specific heat equals to the specific heat of a material. Moreover, with respect to the definition of a heat generation $\dot{Q}$, there is no solid fraction change when the material does not change its state. Therefore, Equation (5.6) can be obtained just with the direct substitution of c_{eff} into an Equation (5.1). During the phase change $\dot{Q}$, as well as, c_{eff} contain terms of latent heat L_f and the solid phase fraction f_s and after substitution of c_{eff} into Equation (5.1) Equation (5.6) is obtained.

Effective specific heat

The effective specific heat c_{eff} of a phase changing materials is often estimated experimentally. Figure 5.2 shows its general relation to the temperature for a phase changing materials.

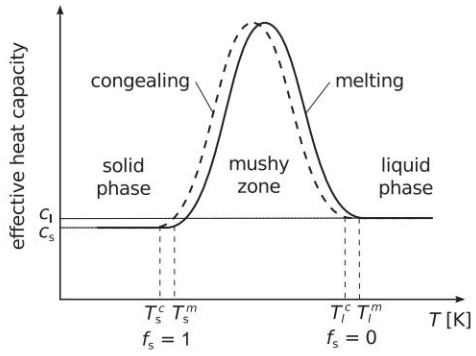

Figure 5.2: Effective heat capacity [15]

In general, the specific heat of solid, denoted as c_s in Figure 5.2, and the specific heat of liquid c_l can differ. Between them a zone where the effective specific heat nonlinearly varies is called mushy zone. Both liquid-phase and solid-phase coexist in mushy zone or in the other words, it is a region where the solid fraction satisfies $0 < f_s < 1$ [15].

It is common for many phase changing materials that a hysteresis occurs. This phenomena provides two solidus temperatures T_s^c, T_s^m and two liquidus T_l^c, T_l^m as it is shown in Figure 5.2. One of these two is specified for the melting and another one for the congealing (solidification). If the hysteresis is not negligible two effective specific heat curves have to be modelled. It complicates the numerical modelling, in consequence of what the condition of a complete phase change should be satisfied before an execution of a backward phase change [15].

For a numerical simulation a time step should be adapted to obtain realistic results during a phase change. A big time step can cause a "jump" over a whole or a large part of a mushy zone in a one step which significantly violates the obtained solution.

An effective specific heat can be described also with a piecewise linear functions or any other function as well, however, the usage of a Gaussian function with a peak in the middle of the phase-changing temperature interval with an appropriate chosen standard deviation is often preferable. Independently on the used function, they should have in the common that a surface under this function equals to the latent heat of a phase change.

6. Numerical methods

The heat transfer problems can be as many other engineering problems studied analytically, experimentally, or numerically.

An analytic method has the biggest disadvantage in its limitation to simplicity. Heat transfer problems are studied on different geometries and even small complication can lead to unsolvability. The boundary conditions difficulty or time variability of some properties are some others examples of its limitations.

Experiments are very expensive and also demand a lot of time and presence of stable conditions, if it is necessary. On the other hand, problem is monitored under real physical conditions and measured quantity error depends only on the measurement accuracy.

Exponential growth of the computational power allows more and more complex problems to be studied numerically. Even though, the studied problem is also simplified to decrease the computational time. Despite that, to discuss and modify a given problem it is more useful to use a numerical method to obtain a sufficiently precise solution. When a behaviour of the problem is not completely predictable, the combination of an experiment and a simulation is a very appropriate choice. With the results obtained from the experiments it is easier to specify the functionality of a numerical model.

An approximated solution of a partially differential equations like the heat transfer problem can be obtained by several techniques. A finite difference method is considered for the next section.

6.1. Finite difference method

A finite difference method as any other numerical method differs from the analytical solution in a continuity. In the beginning the appropriate subdivision of a domain into rectangular areas is chosen as shown in Figure 6.1. The point in the center of this region is called a nodal point or a node and represents a certain region. The functions are evaluated in these discrete points and their values represent an average functional values of a region. The set of nodal points is called mesh or a grid. Increasing the number of the nodal points creates finer mesh and provides more precise approximation.

Let the distance between two adjacent nodal points in a direction of an axis x be Δx and similarly Δy for y space coordination. Nodal point with the coordinates $x = m\Delta x$ and $y = n\Delta y$ will be denoted by (m, n). Moreover, time-dependent problem contains Δt that is the length of a time step between two adjacent discrete times.

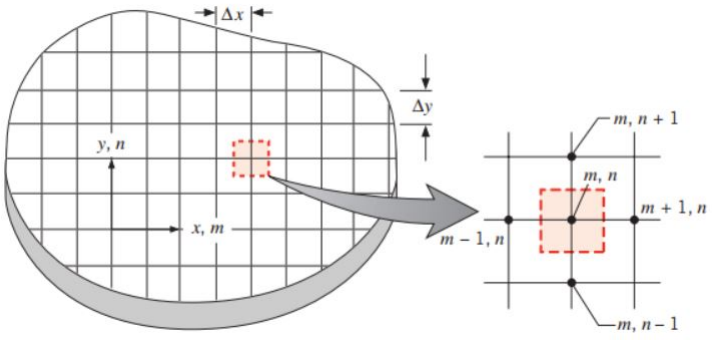

Figure 6.1: Two-dimensional mesh [2]

The idea of the finite difference method is based on a replacement of the derivatives with finite differences. This approximation is obtained from the Taylor series expansion.

Laplace equation

Consider two-dimensional Laplace equation

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0 \tag{6.1}$$

and let $T_{m,n}$ be the temperature at a nodal point (m, n). Then central finite differences of function T at points $x = m - 1/2$, $y = n$ and at $x = m + 1/2$, $y = n$ are

$$\left.\frac{\partial T}{\partial x}\right|_{m-\frac{1}{2},n} \approx \frac{T_{m,n} - T_{m-1,n}}{\Delta x} \qquad \left.\frac{\partial T}{\partial x}\right|_{m+\frac{1}{2},n} \approx \frac{T_{m+1,n} - T_{m,n}}{\Delta x} \tag{6.2}$$

Similarly the second order central finite difference of function T for a nodal point (m, n) can be calculated using last results

$$\left.\frac{\partial^2 T}{\partial x^2}\right|_{m,n} \approx \frac{\left.\frac{\partial T}{\partial x}\right|_{m+1/2,n} - \left.\frac{\partial T}{\partial x}\right|_{m-1/2,n}}{\Delta x} \tag{6.3}$$

$$\left.\frac{\partial^2 T}{\partial x^2}\right|_{m,n} \approx \frac{T_{m+1,n} - 2T_{m,n} + T_{m-1,n}}{(\Delta x)^2} \tag{6.4}$$

The same principle can be used to evaluate finite difference of second partial derivative with respect to y

$$\left.\frac{\partial^2 T}{\partial y^2}\right|_{m,n} \approx \frac{T_{m+1,n} - 2T_{m,n} + T_{m-1,n}}{(\Delta y)^2} \tag{6.5}$$

For a square mesh ($\Delta x = \Delta y$) Laplace equation is in a finite difference formulation for a nodal point (m, n) expressed like a simple algebraic equation

$$T_{m+1,n} + T_{m-1,n} + T_{m,n+1} + T_{m,n-1} - 4T_{m,n} = 0 \tag{6.6}$$

This method is however very limited and a better approach has to be done. The next section introduces the energy balance method that provides identical results but is more widely applicable.

6.2. Energy balance method

Energy balance is based on applying the conservation of energy to a control volume over the nodes [3]. Often requirement from the numerical method is a possibility to work with the material whose properties vary with position. The main advantages of this method are the possibility to handle these more complicated materials and the uncomplicated work with the boundary conditions. Energy balance or also called energy conservation was discussed in Chapter 2.5.

6.2.1. Two-dimensional transient heat conduction

Assume a meshed two-dimensional area where distance between two adjacent nodal points in a one direction equals Δx, for another one it is Δy and a unit depth is assumed. Also consider two-dimension heat transfer negligible in the direction of the unit depth. Moreover, for transient heat transfer the time discretization with time step Δt is considered.

Internal nodes

Assume that this meshed area contains a solid material inside which the heat is transferred by a conduction with a convection heat transfer on its surface. Application of the energy balance on a general interior point *(m,n)* with coordinates is shown in Figure 6.2 where arrows represent the heat flow from adjacent nodes. Temperature in a node *(m,n)* at a time $i\Delta t$ will be noted as $T^i_{m,n}$. $T^0_{m,n}$ is understood as an initial condition.

It is convenient to assume that the heat flows into the node[1] from any direction, which means that amount of the heat leaving the control volume equals zero. Using this fact and knowledge from Chapter 2, energy conservation Equation (2.18) can be rewritten in the form [3]

$$\dot{E}_{in} + \dot{E}_g = \dot{E}_{st} \tag{6.7}$$

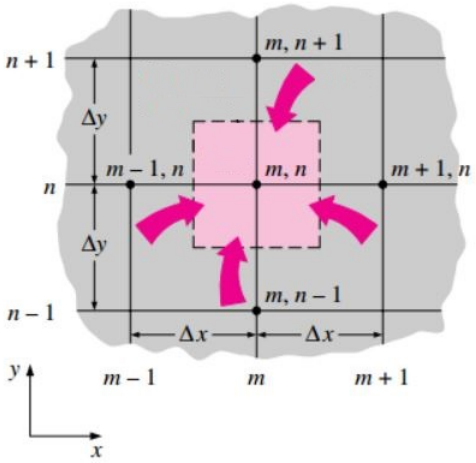

Figure 6.2: Energy balance for a node (m,n) [3]

The goal of this section is to find a proper method to solve numerically Equation (5.6) from Chapter 5. This equation does not contain any heat generation term, therefore the term expressing the rate of a heat generation in last equation has null value. This means that the conservation of energy for a certain studied problem can be expressed as

$$\dot{E}_{in} = \dot{E}_{st} \tag{6.8}$$

Energy transferred inside a control volume of an internal node is caused by conduction from four adjoining nodes. Previous formula can be rewritten as follows

$$\dot{Q}_{cond,left} + \dot{Q}_{cond,right} + \dot{Q}_{cond,up} + \dot{Q}_{cond,down} = \dot{E}_{st} \tag{6.9}$$

where a subscript gives an information about the heat transfer mode and a surface location through which is heat transferred.

[1] The reason for that is almost always unknown direction of the heat flow

Forward difference method can be used to approximate differential equation for a nodal point (m, n). The rate of heat conduction through left (or similarly for right) surface of a nodal point (m, n) is expressed by Fourier's law

$$\dot{Q}_{cond,left}\Big|_{m,n} \approx kA_c\frac{T^i_{m-1,n} - T^i_{m,n}}{\Delta x} = k\Delta y\frac{\Delta T}{\Delta x}, \tag{6.10}$$

where the cross-sectional area A_c in this case equals to the product of height increment Δy and unit depth. It is assumed from the beginning that $\Delta x, \Delta y$ are small enough to obtain a physically accurate solution. Under this assumption a linear temperature variation between the adjoining nodes is not misrepresenting. Clearly, the heat transfer rates become more accurate with finer mesh.

Similarly for the heat conduction from the node on the vertical line

$$\dot{Q}_{cond,up}\Big|_{m,n} \approx kA_c\frac{T^i_{m,n+1} - T^i_{m,n}}{\Delta y} = k\Delta x\frac{\Delta T}{\Delta y} \tag{6.11}$$

The rate of change of the stored energy in a control volume $\dot{E}_{st}$ can be expressed as

$$\dot{E}_{st}\Big|_{m,n} \approx \frac{\rho V_{control}c_p(T^{i+1}_{m,n} - T^i_{m,n})}{\Delta t} = \frac{\rho V_{control}c_p\Delta T_{m,n})}{\Delta t} \tag{6.12}$$

Equation (6.9) is then modified into

$$\begin{aligned} k\Delta y\frac{T^i_{m-1,n} - T^i_{m,n}}{\Delta x} + k\Delta y\frac{T^i_{m+1,n} - T^i_{m,n}}{\Delta x} + k\Delta x\frac{T^i_{m,n+1} - T^i_{m,n}}{\Delta y} + \\ + k\Delta x\frac{T^i_{m,n-1} - T^i_{m,n}}{\Delta y} = \frac{\rho V_{control}c_p(T^{i+1}_{m,n} - T^i_{m,n})}{\Delta t} \end{aligned} \tag{6.13}$$

In the case of a forward finite difference method is called explicit energy balance [2]. However, for an energy balance method also a backward difference can be used and obtained method is called implicit energy balance

$$\begin{aligned} k\Delta y\frac{T^{i+1}_{m-1,n} - T^{i+1}_{m,n}}{\Delta x} + k\Delta y\frac{T^{i+1}_{m+1,n} - T^{i+1}_{m,n}}{\Delta x} + k\Delta x\frac{T^{i+1}_{m,n+1} - T^{i+1}_{m,n}}{\Delta y} + \\ + k\Delta x\frac{T^{i+1}_{m,n-1} - T^{i+1}_{m,n}}{\Delta y} = \frac{\rho V_{control}c_p(T^{i+1}_{m,n} - T^i_{m,n})}{\Delta t} \end{aligned} \tag{6.14}$$

Both of them can be used depending on a problem. The main disadvantage of an explicit method is the step increment restriction and implicit method is harder to implement [3]. The complication in an implicit method is related with the task to solve systems of equations to obtain the new nodal temperature. More about the time step restriction is said in the end of this chapter.

Since the goal is to express unknown temperature at the nodal point *(m,n)* at new time $(i + 1)\Delta t$, the term $T^{i+1}_{m,n}$ can be expressed as

$$T^{i+1}_{m-1,n} = Fo_x\Big(T^i_{m-1,n} + T^i_{m+1,n}\Big) + Fo_y\Big(T^i_{m,n-1} + T^i_{m,n+1}\Big) - T^i_{m,n}\Big(2Fo_x + 2Fo_y - 1\Big) \tag{6.15}$$

where *Fo* is a Fourier number. It is a dimensionless quantity that was already mentioned in the Section 3.2.5. Subscript indicates which spatial increment is used for its calculation and Fourier number for Δx looks like

$$Fo_x = \frac{k\Delta t}{c_p \rho (\Delta x)^2} \tag{6.16}$$

Square mesh simplifies last equation into

$$T^{i+1}_{m-1,n} = Fo\Big(T^i_{m-1,n} + T^i_{m+1,n} + T^i_{m,n-1} + T^i_{m,n+1}\Big) - T^i_{m,n}\Big(4Fo - 1\Big) \tag{6.17}$$

Boundary nodes

Equation (6.13) holds just for any internal node. If the surface temperature is not prescribed, the energy balance for the boundary nodes has to be calculated too. Different types of boundary conditions are explained in section 3.3. With respect to the next chapters of this thesis, convection is the surface condition described in this section.

First configuration of the nodal points on the surface is shown in Figure 6.3. The important remark is that the control volume has half a size in comparison with the control volume of the internal node $V_{internal} = \Delta x \Delta y \cdot 1$. The amount of adjoining nodes

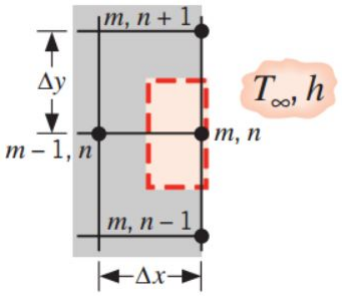

Figure 6.3: Nodal point at the surface with convection boundary condition [2]

from which the heat transfer by conduction occurs is reduced to one internal node and two boundary nodes.

An ambient fluid flow is characterized by an adjoining temperature T_∞ and a convective heat transfer coefficient h. Newton's law of cooling also contains the surface area A, on which the convective heat transfer occurs. For this specific example this surface equals to $A = \Delta y \cdot 1$. Newton's law of cooling then looks like

$$\dot{Q}_{conv,right} = hA\Big(T_s - T_\infty\Big) = h\Delta y\Big(T_s - T_\infty\Big) \tag{6.18}$$

For this boundary condition the energy balance can be expressed as follow

$$\begin{aligned} k\Delta y \frac{T^{i+1}_{m-1,n} - T^{i+1}_{m,n}}{\Delta x} + k\frac{\Delta x}{2}\frac{T^{i+1}_{m,n+1} - T^{i+1}_{m,n}}{\Delta y} + k\frac{\Delta x}{2}\frac{T^{i+1}_{m,n-1} - T^{i+1}_{m,n}}{\Delta y} + \\ + h\Delta y(T_s - T_\infty) = \frac{\rho V_{control} c_p (T^{i+1}_{m,n} - T^i_{m,n})}{\Delta t} \end{aligned} \tag{6.19}$$

Similarly like in the interior node, new temperature for the studied node *(m,n)* can be obtained

$$T^{i+1}_{m-1,n} = Fo_x\Big(T^i_{m-1,n} + Bi_x T_\infty\Big) + \frac{1}{2}Fo_y\Big(T^i_{m,n-1} + T^i_{m,n+1}\Big) - T^i_{m,n}\Big(Fo_x(1 + Bi_x) + Fo_y - 1\Big) \tag{6.20}$$

New dimensionless quantity Bi appears and is called Biot number

$$Bi_x = \frac{h\Delta x}{k} \qquad Bi_y = \frac{h\Delta y}{k} \tag{6.21}$$

For square mesh it is simplified to following form

$$T^{i+1}_{m,n} = Fo\Big(2T^i_{m-1,n} + 2BiT_\infty + T^i_{m,n-1} + T^i_{m,n+1}\Big) - T^i_{m,n}\Big(4Fo + 2BiFo - 1\Big) \tag{6.22}$$

Another and the last type of a boundary condition discussed in this thesis is shown in Figure 6.4 below. Volume is again reduced and equals to $V = \frac{\Delta x}{2}\frac{\Delta y}{2}$. No new concept is

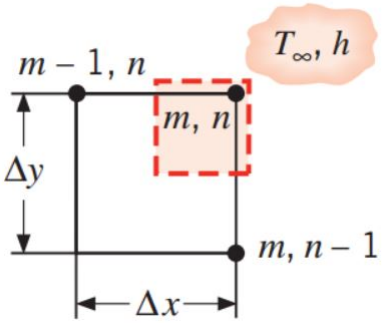

Figure 6.4: Nodal point at the corner with convection boundary condition [2]

used in this boundary condition so he energy balance form can be directly mentioned

$$\begin{aligned} k\frac{\Delta y}{2}\frac{T^{i+1}_{m-1,n} - T^{i+1}_{m,n}}{\Delta x} + k\frac{\Delta x}{2}\frac{T^{i+1}_{m,n-1} - T^{i+1}_{m,n}}{\Delta y} + h\frac{\Delta y}{2}(T_s - T_\infty) + \\ + h\frac{\Delta y}{2}(T_s - T_\infty) = \frac{\rho V_{control} c_p (T^{i+1}_{m,n} - T^i_{m,n})}{\Delta t} \end{aligned} \tag{6.23}$$

Similarly, a more useful form that contains actualized temperature for square mesh can be expressed as

$$T^{i+1}_{m,n} = 2Fo\Big(T^i_{m-1,n} + 2BiT_\infty + T^i_{m,n-1}\Big) - T^i_{m,n}\Big(4Fo + 4BiFo - 1\Big) \tag{6.24}$$

Stability criterion

As it was mentioned above, the explicit method is not unconditionally stable. Stability requires appropriate choice of the time step length. The goal is to choose as big time step as possible, because otherwise the computational time would be unnecessarily huge. If the time step is bigger than the stability criterion a unreal temperature oscillation trough space and time occurs [3].

Assume $T^{i+1}_{m,n}$ is calculated. Stability criterion requires that the sum of all coefficients of $T^i_{m,n}$ is equal or greater than zero [3]. The internal node with a square mesh described by Equation (6.15) is considered

$$T^{i+1}_{m-1,n} = Fo\Big(T^i_{m-1,n} + T^i_{m+1,n} + T^i_{m,n-1} + T^i_{m,n+1}\Big) - T^i_{m,n}\Big(4Fo - 1\Big) \tag{6.25}$$

then the stability criterion is satisfied if $(4Fo - 1) \geq 0$, which implies

$$Fo = \frac{k\Delta t}{c_p \rho (\Delta x)^2} \leq \frac{1}{4} \tag{6.26}$$

Since Δx is fixed and other properties are also known, it is possible to express the inequality for Δt. However, the stability criterion must hold for any node and the most limited inequality has to be taken for a time step length. For example, Equation (6.22) that represents node at a surface with convection boundary condition has more complicated stability criterion

$$(4Fo + 2BiFo - 1) \geq 0 \tag{6.27}$$

that leads to

$$Fo = \frac{k\Delta t}{c_p \rho (\Delta x)^2} \leq \frac{1}{2(2 + Bi)} \tag{6.28}$$

Results verification

Results should be checked for a correctness and an accuracy. For very simple heat transfer problems solution can be compared with analytic solution. Obviously, it is unreal for many problems.

More practical possibility is to apply an energy balance for some properly chosen bigger aggregations of nodal points. Obtained temperatures inserted into energy balance should lead into sufficiently precision. Equality between obtained numbers calculated on a both sides of an energy balance after substituting temperature is not necessary, however, a high precision is required. If this precision is not obtained, it does not directly signify a wrong code implementation. A badly chosen mesh can also has considerably impact into obtained solution. A problem is called a grid-independent when a finer mesh does not provide improvement in an obtained solution.

Afterwards the appropriate choice of the assumptions should be checked. The most easy way to do it is a verification with an experimental data. The numerical model can be executed with different parameters and different assumptions and the similarity with the experimental data can be monitored.

7. Optimization

7.1. Introduction

For many fields from economy up to the industry the optimization is a daily key for their success. Whenever the goal is to find the best possible solution respecting some constraints, the optimization is used. Nowadays the optimization is a discipline between math and computer science, which is still a field with inventing many new approaches.

From the mathematical point of view, the optimization is a searching of the extreme points of a given function called *objective function* in a domain that can be bounded by the constraints given by the equalities and the inequalities. Therefore, an optimization can be considered as constrained if the constraints are given and as unconstrained otherwise. Another classification of an optimization problem is by the linearity – if all functions (objective function and constraints) are linear, the problem is called linear optimization or also linear programming. The problem of finding the minimum of a nonlinear function under constraints is mathematically given in the next definition.

Definition 7.1.1. *A nonlinear minimization problem of an objective function* $f : \mathbb{R}^n \to \mathbb{R}$ *is of the form*

$$\begin{aligned} \underset{\mathbf{x}}{\textit{minimize}} \quad & f(\mathbf{x}) \\ \textit{subject to} \quad & g_i(\mathbf{x}) \leq 0,\ i = 1, \ldots, m \\ & h_j(\mathbf{x}) = 0,\ j = 1, \ldots, p \end{aligned} \tag{7.1}$$

where $\mathbf{x} \in X \subset \mathbb{R}^n$, $g_i : \mathbb{R}^n \to \mathbb{R}$ *for each* $i \in \{1, .., m\}$ *and* $h_j : \mathbb{R}^n \to \mathbb{R}$ *for each* $j \in \{1, .., p\}$, *where at least of one the mentioned functions is nonlinear [25].*

It should be noted that any problem of finding the maximum can be converted by the duality principle into a minimization problem [26].

$$\min_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{x}) = -\max_{\mathbf{x} \in \mathbb{R}^n} (-f(\mathbf{x})) \tag{7.2}$$

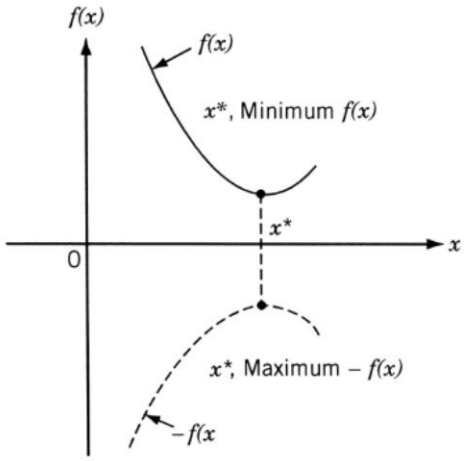

Figure 7.1: Graphical illustration of Equation (7.2) [26]

When a domains of the functions are some subsets of integer numbers, the optimization is called integer programming. The special subcase is a binary programming.

The terminology for the points that are being solutions for a given problem is stated in the next definition.

Definition 7.1.2. *Any point satisfying the constraints is called a feasible point. The set of all feasible points*

$$\left\{x \in \mathbb{R}^n : g_i(\mathbf{x}) \leq 0, h_j(\mathbf{x}) = 0, i \in \{1, .., m\}, j \in \{1, .., p\}\right\}$$

is called the feasible set [25].

If an analysed problem contains the nonlinearities, it is advantageous if the nonlinearity has not a crucial meaning and can be neglected. Mainly because the nonlinear programming is in general much more difficult and the time consuming problem than the linear optimization.

The main problem with the nonlinear optimizations is their behaviour. The numerical methods used for the minimization of a function works with the sufficiently big amount of information[1] to find a local minimum, however, a global minimum is not guaranteed.

Definition 7.1.3. *Let* $\mathbf{x}$ *be a feasible point for a given objective function* $f(\mathbf{x})$ *and its constraints (if are given).*

1. $\mathbf{x}^*$ *is called a global minimum if* $f(\mathbf{x}^*) \leq f(\mathbf{x})$ *for every feasible point* $\mathbf{x}$
2. $\mathbf{x}^*$ *is called a local minimum if exists* $\varepsilon > 0$ *such that* $f(\mathbf{x}^*) \leq f(\mathbf{x})$ *for every feasible point* $\mathbf{x} \in B(\mathbf{x}^*, \varepsilon) = \{\mathbf{y} \in \mathbb{R}^n : 0 \leq \ \|\mathbf{x}^* - \mathbf{y}\| < \varepsilon\}$

Furthermore, the nonlinear constraints can lead to the disconnected feasible regions, which make finding of a minimum much more complicated.

The choice of an initial point has also an impact on the solution. A starting point is closely associated with the difficulties of the nonlinear functions mentioned above - when it is chosen close to the local minimum, there is a fairly big probability that the algorithm will end at that local minimum. Even worse case would be the situation when the nonlinear constrains create the disconnected feasible regions. An every region has its own local minimum and a chance that the algorithm stays only in the one region – the starting one – is very big. Trying more starting points can help to improve the value of an objective function. However, finding more (or even one) initial points can already cause some difficulties [27].

Furthermore, different algorithms have various methodologies for a finding the solution, and as the outcome different results can be produced. Even an one algorithm can provide incomparably diverse solutions for various choices of its parameters.

As it is shown above, it is a hard task to find the solution, however it is still solvable. Chances can be increased by a model simplification or by the restriction of a variable domain. Also, a full understanding of a problem should help to choose a better initial point and a suitable algorithm.

[1] Value of an objective function at a current point (if method uses memory also an information about all visited points is given), gradient and Hessian

7.2. Classification

Before an optimization of a problem, the requirement for a precise optimized solution has to be taken into consideration. If the complexity and difficulty cause the inability to solve the problem in a reasonable time, approximate algorithms can be used. One way of the optimization method classification is shown in Figure 7.2 [28].

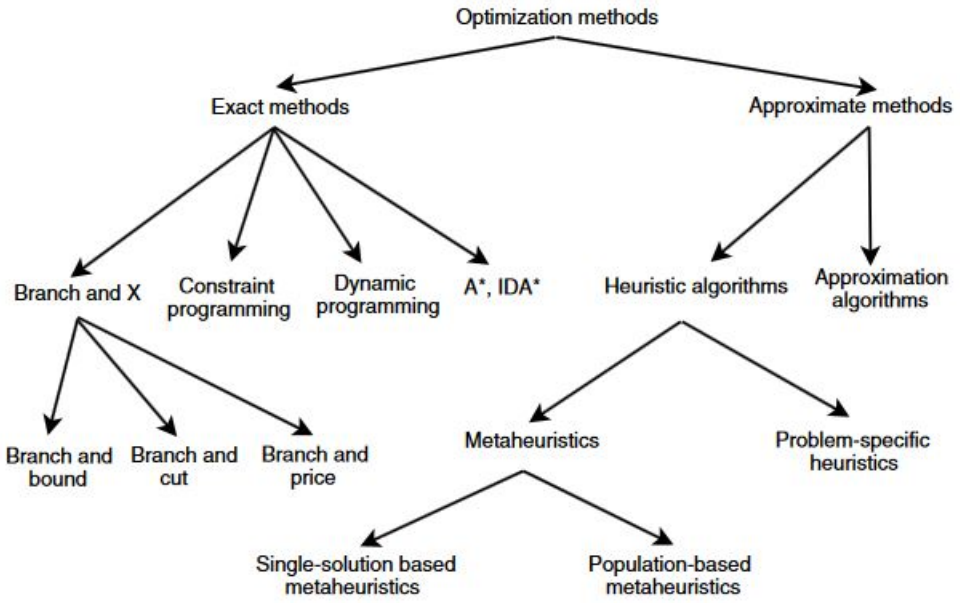

Figure 7.2: Optimization methods [28]

The exact methods also called complete algorithms provide the finding of a precise optimum. The right branch of this graph splits into approximation algorithms, which define how close are the optimal solution and the obtained results, and the heuristic algorithms. The special subclass of the heuristic algorithms are the problem-specific heuristics, which are the problem-dependent techniques. They are usually fitted into the specific problem and work with the certain problem specifications [28].

The metaheuristics are on the other hand problem-independent and therefore suitable for various optimization problems. Their power is based on the effective space searching for big domains. In the last three decades many effective algorithms were developed which led into a popularity increase in a wide range of applications.

The majority of the metaheuristics is inspired by biology and by the nature in general. The well-known algorithms are a genetic algorithm, an evolution of species, an ant colony or a particle swarm. The nature-based algorithms are in general stochastic. For example the local search and the tabu search belong into the deterministic algorithms. The randomness can help them to escape from the local minimum. It should be noted that it implies that the solutions of stochastic algorithms can differ for the same initial settings.

The metaheuristics can be furthermore classified as the single-solution based or as the population based metaheuristics. The first one works with one feasible solution which is tried being optimized. The population-based model keeps a sample of an appropriate solutions and manipulates with them.

7.3. Genetic algorithms

The full advantage of the computational power is needed for many engineering problems. Therefore, a simulation is created to approximately express a real-life problem. When the lack of information of a system behaviour is obtained, the system can be called a black box. A black box can be represented by a black box function with an unknown analytical form. The simulation inputs can be either continuous or discrete and are taken as the function arguments. The function values for those specific arguments are given as the numerical simulation response.

Typical examples of black boxes are the code libraries without any access, the numerical simulation or even the laboratory experiments such as chemical reactions. Even though, when the access into numerical model is available, the complexity and the difficult analysis can make it a black box.

To optimize the black box functions, various combination of input parameters and their behaviour have to be considered. With no internal information or an analytical expression of an objective function, one possible way to solve it is with the metaheuristics. A genetic algorithm was chosen for this thesis [29].

7.4. Fundamental principles

A genetic algorithm is a population-based metaheuristic iterative method that is a subclass of the evolutionary algorithms. As a result of its inspiration by genetic and the natural selection principles also the terminology for these algorithms are copied from the biology terminology. This section is mainly based on [30] and [31].

Assume a binary minimization problem with an objective function $f : \{(0,1)\}^k \to \mathbb{R}, k \in \mathbb{N}$, and $\mathbf{x} = (x_1, x_2, ..., x_n) \in \{(0,1)\}^k$.

An every possible solution $\mathbf{x}$ of this problem is called an individual. The individual is specified by its chromosome $(x_1, x_2, ..., x_n)$ and each component x_i is called a gene. A gene carries some specific information that is called allele[2]. An individual collection of alleles is called genotype. A set of individuals creates a population P and the population size is the cardinality of this set P

$$P = \{\mathbf{x_1}, \mathbf{x_2}, ..., \mathbf{x_N}\}$$

As a fitness function is understood any function that measures a fit of an individual. A value of fitness function for an individual is called fitness[3]. The choice of a fitness function depends on the nature of the problem and the objective function can be chosen as well.

In [31] was a fitness function F chosen as follows

$$F(\mathbf{x}) = \frac{F_{max} - F_{min}}{f_{min} - f_{max}} f(\mathbf{x}) + \frac{f_{min}F_{min} - f_{max}F_{max}}{f_{min} - f_{max}} \tag{7.3}$$

[2]In this case a gene gives information that it contains binary variable and its value (either 1 or 0) is allele

[3]In [28] is used term fitness for a function and fitness value for function value of an individual

where f_{min} and f_{max} is the smallest and the biggest objective function value for the individuals in the population. F_{max} and F_{min} are chosen values usually $F_{max} = 1$ and $F_{min} = \varepsilon$, where ε is small enough, e.g. $\varepsilon = 0.01$ [31].

This function can be furthermore normalized

$$F'(\mathbf{x}) = \frac{F(\mathbf{x})}{\sum_{j=1}^{N} F(\mathbf{x_j})} \tag{7.4}$$

which can be interpreted as a probability of a given individual for a reproduction of his genetic information, i.e. to make a child.

The reproduction is one of the genetic operations and they are discussed in the next sections.

7.4.1. Selection

Selection is a methodology to choose two convenient individuals for the next generation of a population. The principle of a natural selection is applied for the selection. The individuals with better fitness have in general higher probability to be selected, but the element of randomness is also present in many of these methods.

There exists different ways to select individuals appropriate for the reproduction. One of the most used methods is a Roulette selection, when a probability of choosing some individual is proportional to its fitness. From two chosen individuals called parents two children are made by reproduction.

Another similar method also inspired by the nature is the competition between two or more random individuals. The one with higher fitness becomes the child in the next population.

Another way is to neglect the stochastic impact and the individuals with the highest values can be directly chosen as parents. The individuals with the highest fitness values are called elites. In a method called elitism is the elite individual directly moved into the new population. More examples can be found in [30].

7.4.2. Reproduction

The reproduction operator or also called a crossover is a method of merging parental genes. It is based on an assumption that the quality of a fitness of the parents should be hereditary to the children.

The most common method is the one-point crossover. For two selected parents $\mathbf{x} = (x_1, x_2, ..., x_n)$ and $\mathbf{y} = (y_1, y_2, ...y_n)$ a random number k, such that $0 \leq k \leq n$ is uniformly chosen. Then two children $\bar{\mathbf{x}}$ and $\bar{\mathbf{y}}$ are made by a following scheme

$$\bar{\mathbf{x}} = (x_1, x_2, ..., x_k, y_{k+1}, ..., y_n)$$
$$\bar{\mathbf{y}} = (y_1, y_2, ..., y_k, x_{k+1}, ..., x_n)$$

Similarly a two-point crossover can be done, where two random numbers k, l, such that $0 \leq k < l \leq n$ are uniformly chosen. Two children are made by swapping parental genes between them

$$\bar{\mathbf{x}} = (x_1, x_2, ..., x_k, y_{k+1}, ..., y_l, x_{l+1}, ..., x_n)$$
$$\bar{\mathbf{y}} = (y_1, y_2, ..., y_k, x_{k+1}, ..., x_l, y_{l+1}, ..., y_n)$$

7.4.3. Mutation

The evolution of a population is also affected by a mutation. the mutation is a change of one or more genes to some random values. This randomness ensures diversity and can help not to stuck in a local minimum. The probability of a mutation should be chosen very small.

In a Bit-flip mutation a random number k_i, such that $0 \leq k_i \leq 1$ is generated for every gene of an individual. If a Bit-flip mutation parameter of the probability p holds $p \geq k_i$ negation is used on i-th component [30].

7.4.4. Representation

The binary representation that is used in this section represents the individuals as a bit string. The classical example is a Knapsack problem [32] which can be solved with boolean variables. For finding a minimum of a function, genes of an individual can store the space coordinates for a possible solution. However, these numbers should not be converted into their binary representation directly, but another methodology should be used.

For example, considering a decimal number 8 that can be binary represented[4] by 1000 and a decimal number 7 decoded to 0111. Their Hamming distance[5] is three, which is big with comparison to the string length. To obtain 8 from 7 by mutation, all four bits have to flip. With a small mutation rate the change in every bit is almost impossible. Furthermore, consider that a population contains only individuals encoded to 01**, where symbol * can obtain values 0 and 1. It is not possible to obtain 8 even with the crossover operator. Another case is when the similar genotype (i.e. genotype 1001) is in a population but has inappropriate fitness and therefore it will not be selected for the reproduction [30].

This occurrence called the Hamming cliff [33] happens when the sufficiently close phenotypes or a bad fitness lead to a very large change in the genotype [30]. It is possible to avoid the Hamming cliffs with another methodology known as Gray coding. Gray code [34] is a better implementation of a binary code where any two adjacent integer numbers differs in one bit. Small change in the genotypes leads to a better optimization and nowadays almost every binary representation in a genetic algorithms is implemented by the Gray code [35].

For different problems it is appropriate to use different representations. Real valued representation is mostly used when the alleles are real numbers. For discrete values of the alleles an integer representation is also appropriate. For other representations it is required to modify some operator for a better convergence. A good example is the mutation for integer representation where the flipping bits is not possible. Mutation into another randomly chosen numbers is often used.

[4] In another words a decimal number 8 is encoded into genotype 1000. Similarly, genotype 1000 can be decoded into phenotype 8

[5] The number of positions at which codes differ

7.4.5. Algorithm

The initial population has to be chosen at the beginning of the whole process. The main key is to accomplish a diversity in the population. In general, the size of the population is even-numbered for easier manipulation with parents. In general, the population size is not changing and also the individual alleles have the same size, which simplify binary operator – reproduction.

As the stopping criterion can be used the maximal number of generated populations or reaching pre-defined required value of the objective function. Another example is a number of generations without improving fitness of their individuals or the number of the same individuals in the population. Furthermore, the maximal number of generations is often used in a combination with another condition for a stopping criterion.

However, all this concepts are slightly problem-dependent and should be chosen after the problem analysis. The pseudocode of the genetic algorithm is shown bellow.

```
select an initial population
Fitness calculation
while Stopping criterion is not reached
    Selection
    Reproduction
    Mutation
    Fitness calculation for a new population
end
```

7.4.6. Modifications

Up to now, the genetic algorithm was discussed as the unconstrained optimization. That is however limiting and time consuming. Therefore, some methodologies as the penalty function have to be considered for.

With the penalty function [36], the constrained problem is modified into the unconstrained, where to the all constraints violations a penalty is added to the fitness. This penalty decreases a chance of its selection and therefore the chance for another reproduction. Many different penalty functions are developed for the genetic algorithms and they often work reasonably well just for some specific kinds of problems [37] [38].

A repair algorithm is another approach to handle the constraints. When an infeasible solution is found, mostly random change of alleles is used to repair it into the feasible solution. There is a check after each change if the repaired individual belongs to the feasible set, which can be time consuming in some cases [39].

Another approach to handle constraints is by the modification of a genetic algorithm. The genetic algorithm can be modified by its combination with some another method or with a redesign. In the redesign new genetic operators are implemented in such way, that the new individual from these operators is guaranteed to be a feasible solution. In this category the most popular method is the GENOCOP system [37].

8. Model setup of the thermal energy storage unit

This chapter connects all the theoretical knowledge from the previous chapters into the practical problem.

In the first section of this chapter a model setup is discussed that is directly followed by a brief introduction into the computer model ideas and assumptions.

8.1. Model construction

The problem is to optimize the chosen parameters of the thermal energy storage with a phase change material for a better energy storage. The appropriate temperature range allows to the chosen phase change material to store more heat due to the latent heat during the phase change. When all requested parameters are chosen the numerical model that describes the heat flows through the storage unit is constructed. The heat exchange between the air and phase change material is modelled, therefore, this computer model contains the conduction, as well as, the convection.

This whole model is configured with respect to the thermal energy storage unit that was used and described in [15]. The similarity should help to verify obtained result with results obtained in [15].

In this thesis a paraffin-based phase change material RT42 is considered whose properties can be found in [40]. The useful properties for next process are shown in Figure 8.1.

Melting temperature range	38–43 °C main peak 41 °C
Congealing temperature range	43–37 °C main peak 42 °C
Heat storage capacity in temp. range between 35 °C and 50 °C	174 kJ kg^{-1} (±7.5%)
Specific heat in both solid and liquid states	2 kJ kg^{-1} K^{-1}
Density in solid state at 15 °C	880 kg m^{-3}
Density in liquid state at 80 °C	760 kg m^{-3}
Volume expansion in temp. range of phase change	14%
Heat conductivity	0.2 W m^{-1} K^{-1}

Figure 8.1: Properties of RT42 [15]

The paraffin wax is located inside the aluminium compact storage modules (CSM) which provide an easy manipulation with demands on the storage volume or the plates arrangement [15]. In an experiment CSM modules are stored in the TES in the configuration that is shown in Figure 8.2.

The storage unit contains 100 modules arranged in 5 columns and with 20 panels in each column. The dimensions of CSM is 450 mm × 300 mm × 10 mm and the internal storage unit dimensions are 440 mm × 620 mm × 1800 mm [15]. In the direction of the air flow, distance between panels is set to 30 mm and there are 20 mm channels for the air flow between two panels in a direction of a storage unit height. The energy storage with these parameters is shown in Figure 8.3.

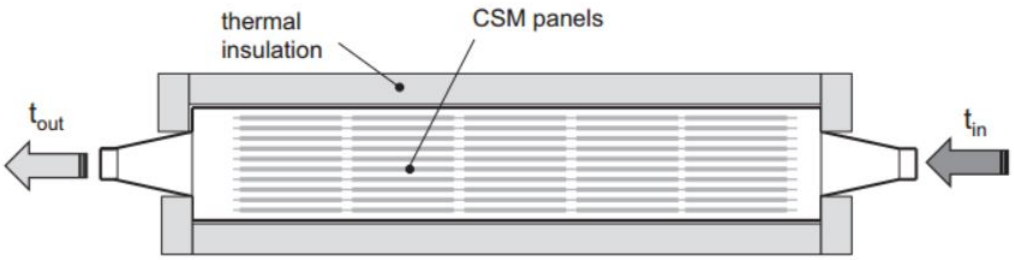

Figure 8.2: Thermal energy storage [15]

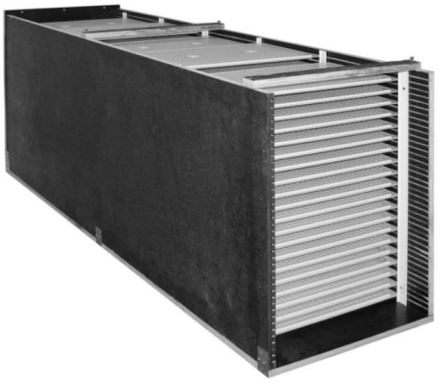

Figure 8.3: Themral energy storage unit without the insulation on two walls [15]

The initial temperature in the whole storage unit is 25 °C. Then a fan situated in the inlet to the thermal energy storage unit with the air flow rate 230 m^3h^{-1} is switched on with almost constant inlet temperature of 58 °C. During this phase the energy is accumulated in the storage unit and after 4 hours the fan switches its temperature into the intial temperature 25 °C. For another 4 hours the heat release is monitored [15].

8.2. Numerical model

An explicit energy balance method described in Section 6.2 is used for a numerical model of the thermal energy storage unit. The temperature in any nodal point of the domain is calculated for each step with equations obtained in Section 6.2. During simulations the phase change of paraffin-wax occurs. The phase change can be easily handled with a specific heat method (Chapter 5). For a RT42 an appropriate Gaussian function can be chosen as follows [15]

$$e_{eff}(T) = 2000 + 5620 \exp\left\{ - \frac{(T - T_m)^2}{2.1} \right\}, \tag{8.1}$$

where T_m is the melting temperature.

For the numerical model following assumptions were considered to obtain simplified version of the real-life problem. The thermal energy storage is totally insulated from the surroundings, therefore no heat loss occurs from the storage unit. The internal flow is simulated as one-dimensional and the convective heat transfer coefficient is calculated from Nusselt number correlations that are chosen from [2]. Furthermore, it is assumed

that flow is fully developed for each air channel between two CSM modules. For the laminar flow Nusselt number is constant

$$Nu = 3.66 \tag{8.2}$$

and for the turbulent flow Nusselt number can be calculated as

$$Nu = \begin{cases} 0.0023 Re^{4/5} Pr^{0.3} & \text{for cooling} \\ 0.0023 Re^{4/5} Pr^{0.4} & \text{for heating} \end{cases} \tag{8.3}$$

where Re is Reynold number and Pr represents Prandtl number.

The air flow scheme for two CSM panels in a direction of the air flow with two horizontally positioned panels is shown in Figure 8.4.

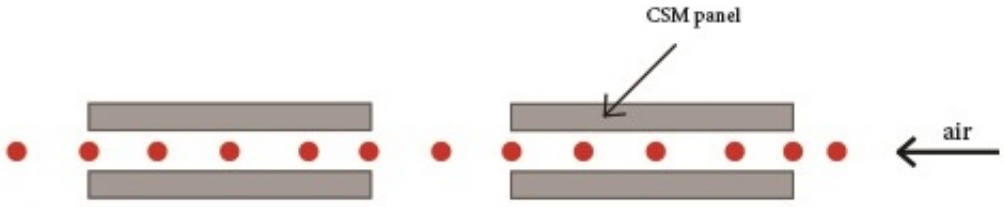

Figure 8.4: Air flow scheme

In the cross-sectional direction the air channel can be represented sufficiently with just one node, because of the constant properties values assumption in channels.

Three nodes with arrows symbolizing the direction of heat transfer and air flow are shown in Figure 8.5. The amount of transferred heat in nodal point n into two panels is expressed by two Newton's law equations

$$Q_{PCM,n1} = \frac{\Delta x}{2} h (T_n - T_{PCM,n1}) \Delta t \tag{8.4}$$

$$Q_{PCM,n2} = \frac{\Delta x}{2} h (T_n - T_{PCM,n2}) \Delta t \tag{8.5}$$

For interior node $n+1$ the difference is only in the area that has double size.

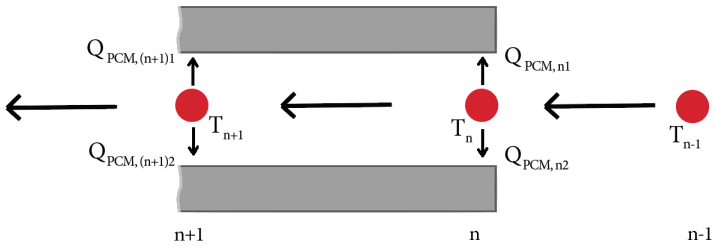

Figure 8.5: Air temperature calculation

For the node $n+1$ is the temperature calculated from

$$\dot{m} c (T_n - T_{n+1}) = Q_{PCM,n1} + Q_{PCM,n2} \tag{8.6}$$

$$T_{n+1} = T_n - \frac{Q_{PCM,n1} + Q_{PCM,n2}}{\dot{m} c_p \Delta t} \tag{8.7}$$

In Figure 8.5 node $n - 1$ does not interact with any CSM panel, therefore, $T_n = T_{n-1}$. When a time dependence is considered, the temperature in node n at time step k is calculated as

$$T_n^k = T_{n-1}^{k-1} \tag{8.8}$$

When the model is assembled the energy balance control can be done. In this control the equality between the amount of the heat that was accumulated in the PCM and the amount of the heat that was released by air for every time step is checked. It can be seen on the obtained results that energy balance is verified for a sufficiently high precision as it is shown in Figure 8.6. The only difference occurs at the beginning when the fan was switched to 58 °C and therefore for a short time period is the temperature at the inlet and at the outlet of the storage unit quite big.

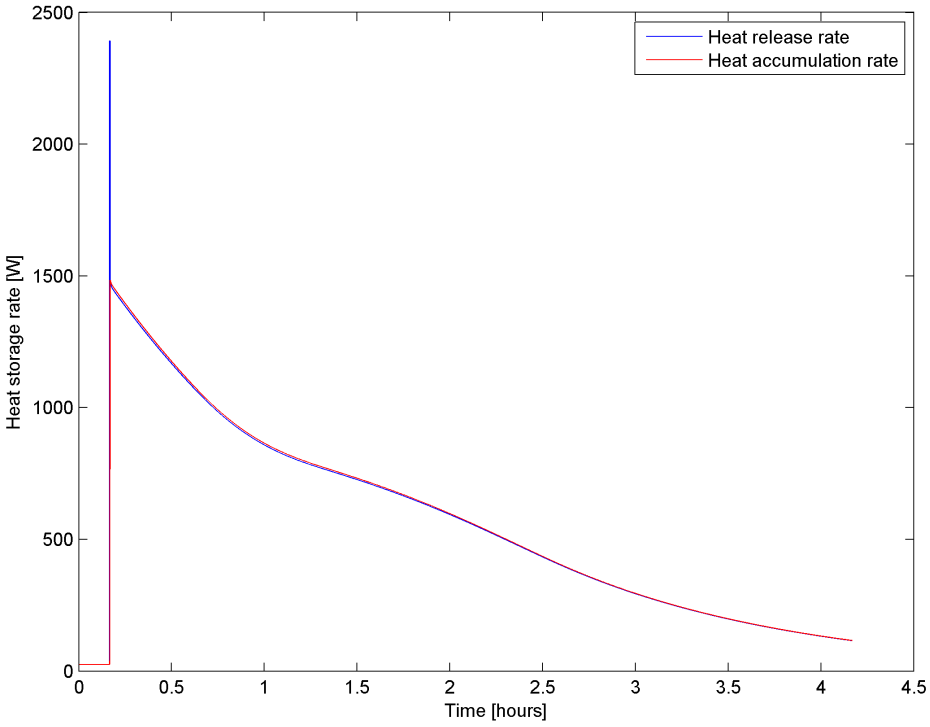

Figure 8.6: Energy balance for TES

Moreover, obtained simulation results are compared with experimental results, as well as, with the numerical results presented in [15]. Obtained results are compared with respect to the obtained or measured outlet air temperature from the thermal energy storage. Three curves – results obtained in this thesis, numerical and experimental results obtained in [15] – are shown in Figure 8.7. For the experiment was harder to obtain an initial constant temperature which leads to 10 minutes delay to achieve this condition. Therefore, numerical methods were also shifted and the heat storage process was from 0:10 hours to 4:15 hours. Then a fan switched its temperature into 25 °C and a heat release period took place from 4:15 hours to 9:00 hours.

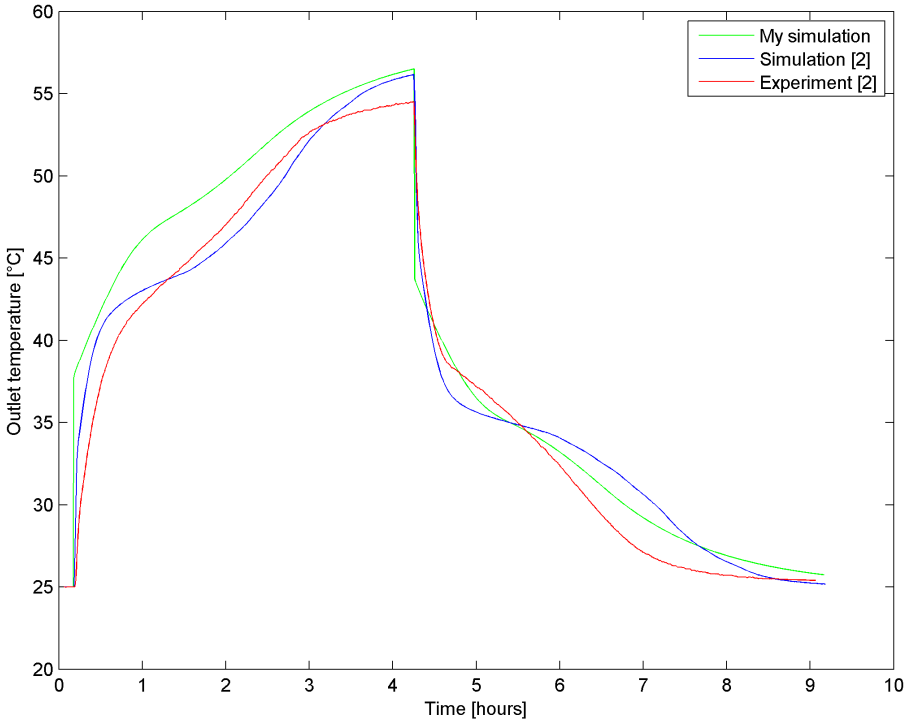

Figure 8.7: Outlet air temperature from thermal energy storage

Results obtained in this thesis have quite similar behaviour with remaining two curves and the model can be considered as verified.

9. Optimization and results

When the computer model is verified it is possible to study the thermal energy storage unit with the goal to increase the amount of stored heat. The amount of stored heat is a function of the temperature with unknown analytical form. Therefore, the lack of information makes this objective function a black-box function. For these types of functions a genetic algorithm is the appropriate choice that is for the aim of this thesis implemented in Matlab. This method is in detail presented also with the pseudocode of this method in Section 7.3.

A genetic algorithm uses several operations – the selection, the reproduction and mutation. The methodologies how to accomplish them are not strictly given and can be chosen with respect to the problem. For this thesis the selection is implemented by a tournament method and also the best individual becomes automatically the individual of the new population by the elitism method. The reproduction is done by one-point crossover method and mutation by a Bit-flip mutation with 0.01 probability rate. Moreover, the initial population is always randomly generated with 12 individuals and the stopping criterion is the combination of the maximal number of generations and the stagnation – when fitness does not improve for 40 generations. For a code implementation the practical and theoretical hints from [30] and [42] are used.

Two design optimization problems are solved in this section. Both of them analysis the appropriate designs of the thermal energy storage and their influence to the accumulated heat. The amount of accumulated heat is chosen as the objective function for its simple representation.

The thermal energy storage in this section is based on the model setup from the previous chapter. However, due to the time difficulty of these problems is more appropriate to model just first four hours – the heat storage period. The effective way how to accelerate the simulation is the *codegen command*. This command rewrite Matlab code into C++ file called *Mex file* that is executable directly from the Matlab but significantly decrease the evaluation time. Even though, the simulation of nine hours is still time-consuming and just four hours are simulated.

9.1. Design optimization of the CSM panels configurations

In the first problem the effects of the various configurations of the plates to the amount of the stored heat are studied. The goal is to design the thermal energy storage that contains maximally 100 CSM panels. The air channel between two plates is always 30 mm and in each row the same number of plates has to be accommodated. Furthermore, at least three plates have to be assembled in each column or in each row of the storage unit to avoid such designs that are extremely occupying the space in the room where the storage unit is situated.

Therefore, the input into the black-box model is given by an ordered pair *(x,y)*, where x expresses the number of rows and y number of columns. The output of a black-box function is the amount of the stored heat with its heat storage rate. When these values are obtained for each individual in a population a genetic algorithm takes place with an

effort to improve the value of the objective function. This process is called simulation in a loop and is shown in Figure 9.1.

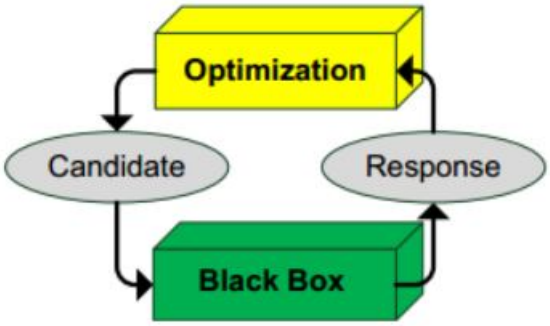

Figure 9.1: Simulation in a loop [29]

This problem belongs to the integer programming, hence the configuration has to be represented by integers. Therefore, the individual in the population can be expressed by its chromosome *(x,y)*, where both genes *x, y* carry the information about the number of plates in their direction. The binary representation with Gray code was used (see Section 7.4.4), mainly for the better diversity for reproduction[1].

With respect to the conditions – at least 3 plates in each direction, at most 100 panels and the same number of plates in each row – it is sufficiently enough to represent each gene by a 6 bit string. The biggest number that can appear in the feasible solutions which satisfies these conditions is 33 – (33, 3) or (3, 33). The Gray code of this number is 110001 and up to decimal number 64 it is possible to express all of them with 6 bits. However, due to the optimization code construction, where inputs are integers, it is appropriate to code and decode between the integers and Gray code every time. Moreover, results are more readable but it increase the chance of finding possible mistake in results.

To satisfy these conditions a repair algorithm is used. For every obtained infeasible solution a random number is added or subtracted, depending on the current position, until the feasible solution is obtained.

Moreover, it is appropriate to save all fitness (values of objective function) to some variable, hence some individuals (feasible solutions) can be applied multiple times.

The amount of the stored heat is evaluated from the heat storage rates that can be expressed as [15]

$$\dot{Q}_{in} = \dot{m} c_a (T_{in} - T_{out}), \tag{9.1}$$

where $\dot{m}$ is the mass flow rate, c_a represents the specific heat of air and T_{in} T_{out} are the inlet and outlet temperatures, where T_{in} is fixed to the constant value 58 °C. By integration with respect to the time variable the stored heat is obtained.

[1]For example, two individuals with chromosomes (7, 5) and (14, 3) respectively, have just one possible option how to combine their genes – new individuals are (7, 3) and (14, 5). On the other hand, for the same two individuals represented by Gray code (0111, 0101) and (1110, 0101) the number of possible combinations increases.

9.1.1. Results

The best obtained solution was (3, 33) – 3 rows and 33 columns. The amount of stored heat is 9.27 MJ and the heat storage rate can be seen in Figure 9.2.

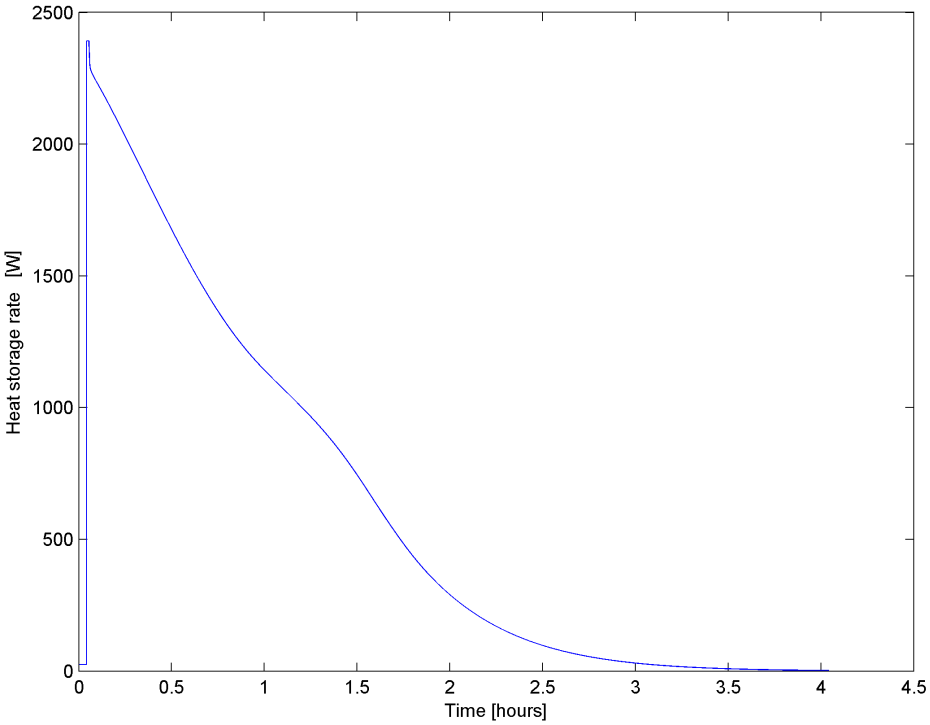

Figure 9.2: Heat storage rate

The solution was found in the 8-*th* generation, however another 40 generations were necessary to successfully stop the algorithm due to the stopping criterion as it is shown in Figure 9.3. The best obtained configurations are summed up in a Table 9.1.

Table 9.1: The best obtained configurations with respect to the amount of stored heat

Rank	Configuration	Stored heat [MJ]
1	(3,33)	9.27
2	(4,25)	9.23
3	(5,20)	9.14
4	(3,32)	8.99
5	(4,24)	8.86
6	(25,4)	8.41
7	(20,5)	8.41
8	(9,11)	8.36
9	(11,9)	8.34

The best results were obtained for a less number of rows and much more columns. It is caused by a fact, that with decreasing the amount of panels in each row the flow rate through the air channels is increasing and amount of the stored heat depends proportionally on the air flow velocity – higher velocities imply higher values of the convective heat transfer coefficient. These results could be effected by the assumption that there is no

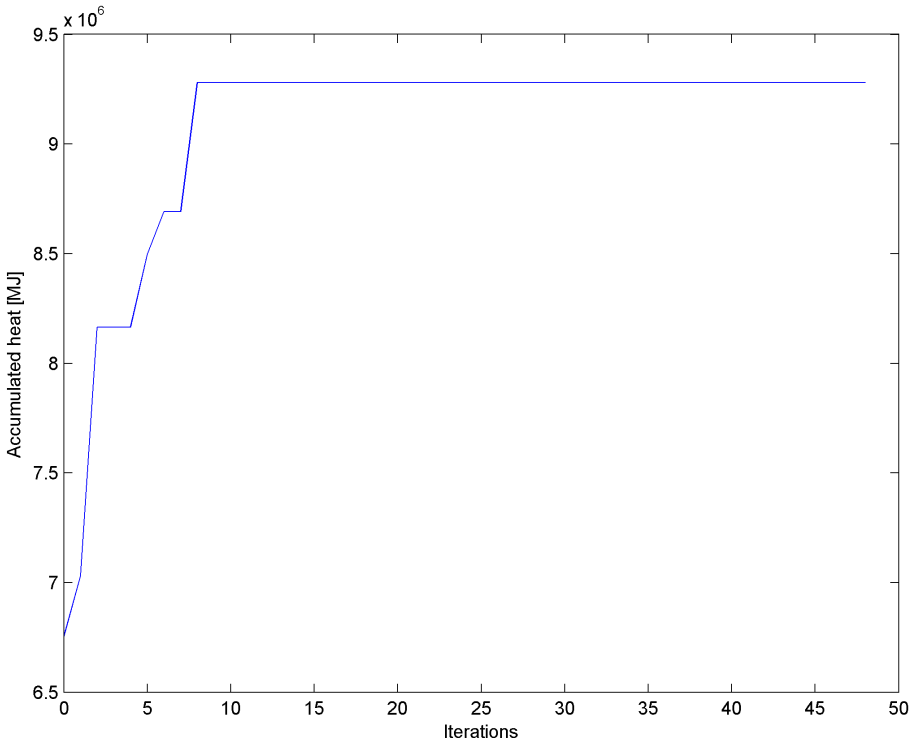

Figure 9.3: A genetic algorithm space search

heat loss in the storage unit, however, in a real-life problem it is possible to accomplish these results with increasing thermal resistance of the walls.

The heat storage rates for some results are shown in Figure 9.4. The rapid increase of the heat storage rate at the beginning of the simulation was caused with different inlet and outlet temperatures up to time when the air flow reached the end of the last panel.

It should be reminded that the genetic algorithm belongs to the approximate methods and the global optimum is not guaranteed. All combinations of plates that were calculated during the optimization process were saved to the text file, therefore, the optimization process could be repeated. For the first time the results were obtained after more than 2 hours. However, hence the results were saved it was possible to execute the optimization model more times to study if it can find better configurations of the plates that were not visited yet. The calculations time dropped to several minutes but a better configuration was not found. However, the text file contained all combinations for at least 80 CSM panels, therefore, a genetic algorithm very deeply searched the region with the highest objective function values and obtained result can be considered as a global maximum.

In Figure 9.5 is the graphical visualisation how a genetic algorithm searched through the space where are marked the best feasible solutions, visited feasible solutions as well as all feasible solutions. This results were obtained for the first simulation during 48 iterations.

One of the advantages of the genetic algorithm is a possibility of a parallel implementation [43]. The time increases nonlinearly with a size of a problem and for a more complex tasks a parallel implementation should be considered.

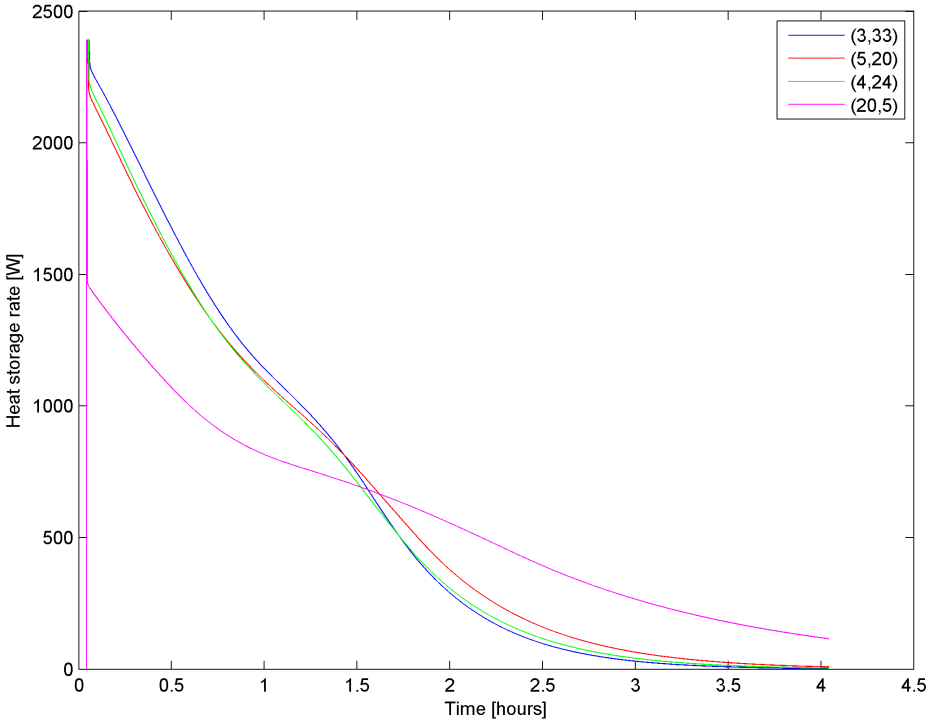

Figure 9.4: Heat storage rates for different configurations

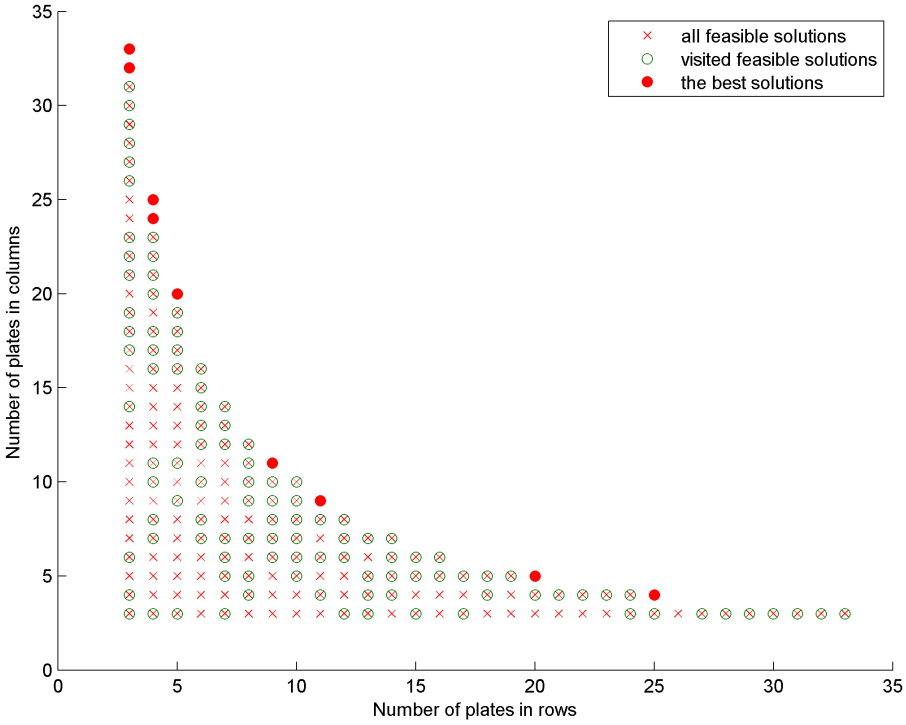

Figure 9.5: Maximal objective function in a given iteration

9.2. Design optimization for various thickness and plates configurations

In the second case a 70 kg of a phase change material is available for a storage unit. The goal is to find the configuration as well as the appropriate panel dimension to maximize the amount of stored heat. Three different types are considered and all of them have two identical dimensions and the third one – thickness – can be chosen. One of these three plates was already used in the first case – 450 mm× 300 mm× 10 mm. The other two plates vary in the third dimension, namely available dimensions are 15 mm and 20 mm. Denote them in order as Plate 1, Plate 2 and Plate 3. The thermal energy storage unit has the same number of plates in each row with at least three plates in both direction. Furthermore, it has to contain all plates of the same thickness, otherwise the problem would be much more difficult.

Plate 1 from the previous example contains about 700 ml of paraffin-waxed material [15]. Therefore, it is possible to fill 100 CSM panels with 70 kg of PCM. At most 66 CSM of Plates 2 can be filled with 70 kg and 50 panels for the case of Plate 3.

The heat storage is represented by the black-box function with three inputs x, y, k, where x is the number of rows, y is the number of columns and k represents the thickness of plates denoted by three integer number – 1, 2, 3 – for easier manipulation. Since there are just three possible plates type, the third input k can obtain just three values. The advantage of this problem is possibility to execute the simulations just for the second and third type of panels, hence for the first type are almost all results already obtained from the previous problem.

On the other hand, just three possible variations of k make the problem more complicated, hence the genetic algorithm should not operate with k as with the other two inputs. The first two inputs can reproduce and mutate on the regular base, however, some variation with bits of third variable can easily produce a different number than 1, 2 or 3. Therefore, the genetic algorithm was modified in a such way that when a new configuration was obtained a simulation was executed for both thickness. Afterwards, the results from the smallest thickness are loaded or computed and one thickness with the better value was inserted into the population and the other two results were just saved. This significantly increased the number of code executions, however, the set of feasible solutions for this problem is quite small.

Similarly with the first case, just 4 hours of heat storage period were simulated to decrease the computational time. Properties of the paraffin-based material as well as all other aspects are the same.

9.2.1. Results

The evaluation time was about an hour and a half and the algorithm was stopped due to the stopping criterion in the 46-*th* iteration. However, it should be reminded that for 40 iterations the maximal value of the objective function was not changed with respect to the chosen stopping criterion.

Even though, the first problem is a subproblem of this one and has less feasible solutions a number of iterations necessary to satisfy its stopping criterion were in general greater than in this problem. It is caused by the modification of the code, when for a given

configuration the most appropriate thickness is chosen. Moreover, the elitism selection was considered, therefore, a lot of suitable individuals survived to the next generation.

The evaluation time is adequate to the fact that for one configuration two or three results were calculated. Moreover, the heat transfer is significant mainly in a direction of the plate thickness and for 20 mm thickness each panel contained twice as much nodal points than 10 mm panels.

The best obtained solution was found for configuration (3, 33, 10 mm) with 9.27 MJ of accumulated heat during four hours. The result is identical with the solution obtained in the first problem. Another obtained results are summed up in a Table 9.2.

Table 9.2: The best obtained results with respect to the amount of stored heat

Thickness [mm]	Configuration	Stored heat [MJ]
10	(3,33)	9.27
10	(4,25)	9.23
10	(5,20)	9.14
15	(3,22)	9.03
15	(5,13)	8.71
15	(4,16)	8.66
20	(5,10)	8.71
20	(4,12)	8.47
20	(3,15)	8.06

The heat storage rates for chosen combinations are shown in Figure 9.6.

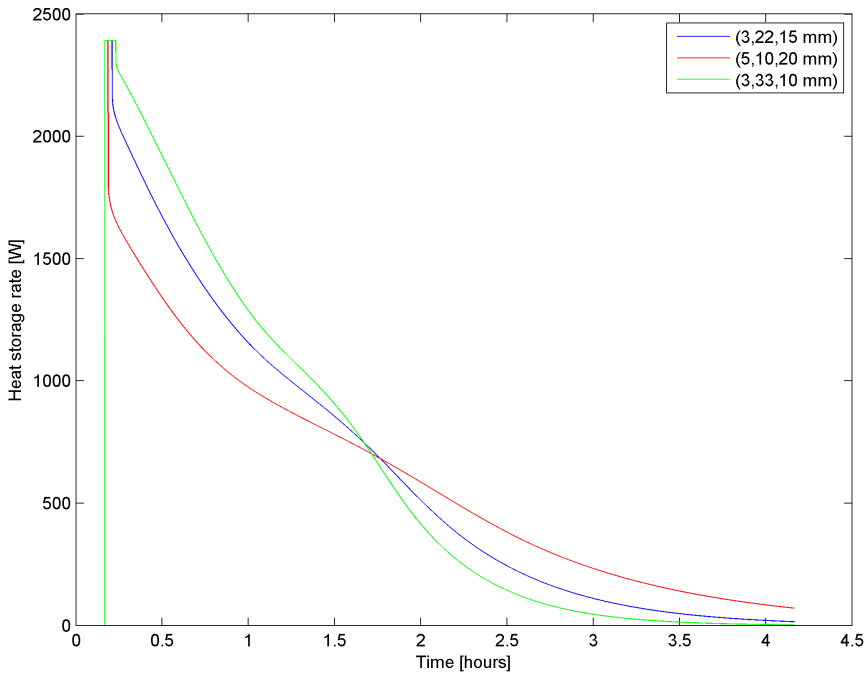

Figure 9.6: Heat storage rates for different configurations and thickness

It can be seen that the thickness 10 mm contains the best results for this problem. It can be caused by a material property – thermal conductivity – that is quite small for

a chosen paraffin RT42. Therefore, the amount of the heat transferred by a conduction is less significant than the heat transferred by a convection what caused a problem for thicker plates.

The shape of the heat storage rates in Figure 9.6 can be explained by a fact that in thinner CSM plates more heat is accumulated from the beginning and therefore also a phase change with an accumulation of the latent heat occurs earlier. As it is shown in Figure 9.7 this behaviour can be viewed also from the outlet temperature from the thermal energy storage where the thinner plate has lower temperature from the beginning – more heat was accumulated.

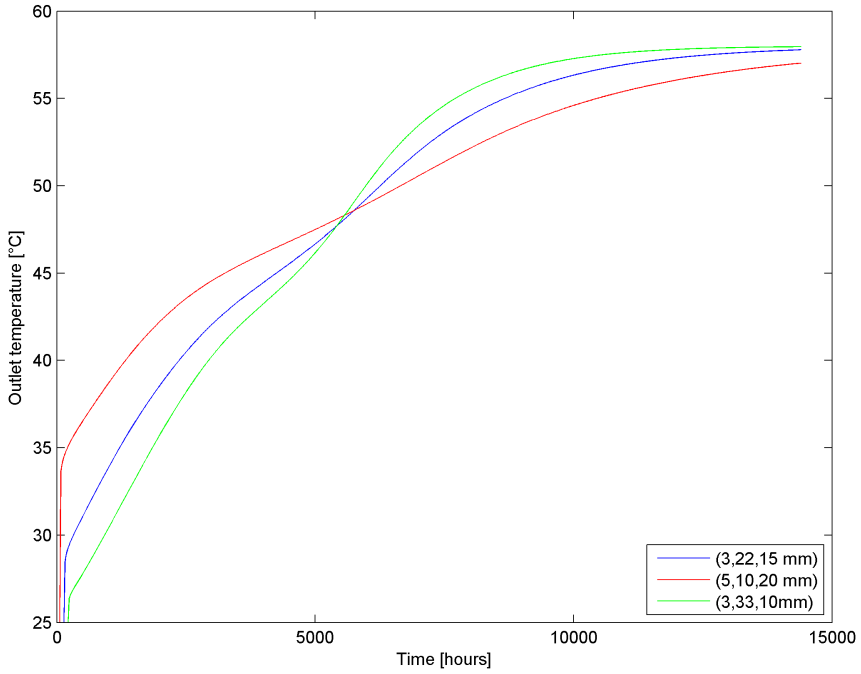

Figure 9.7: Outlet temperatures from the thermal energy storage

Also this problem was solved multiple times, however, the better solution was not obtained. A genetic algorithm precisely searched through the space also in this case and a problem can be considered as a global maximum as well.

Therefore, a genetic algorithm was an appropriate choice for these problems when in both cases found the global maximum. Moreover, the number of iterations was quite small with respect to the studied problem. The time could be decreased even more with choosing more tolerant stopping criterion.

10. Conclusion

This thesis deals with the design optimization of the thermal energy storage. The results presented in this thesis provide information about a behaviour of the stored energy with respect to the configuration of plates assembled inside the storage unit. Moreover, code implemented into Matlab can be modified for another wide spectrum of analysis.

The theoretical background from the first chapters has wide range of applications in various thermodynamics and heat transfer problem. Therefore, in the first part of this thesis the general terminology with deeper analysis of convection and conduction, principles of a thermal energy storage unit and possible methods to store the energy are presented. Afterwards, an appropriate numerical method is chosen and the equations necessary for this method are derived. Also a general introduction into the optimization is given with a description of a genetic algorithm that is suitable for a studied practical part. In the practical part, in Chapter 8, the computer model is discussed with the necessary assumptions and properties used for its implementation into Matlab. Moreover, some additional calculations necessary for the correct implementation are presented in this chapter as well. The functionality was verified and the model was used for optimization in Chapter 9.

In Chapter 9 operations used in a genetic algorithm were briefly mentioned afterwards used for a design optimization of the thermal energy storage. This chapter also contains two problems with a goal to maximize the amount of stored heat which were the main goals of this master thesis. A knowledge from previous chapters was used for a solving and problems were implemented in Matlab, as well.

Both optimization problems belong to the constrained integer programming with non-linear objective function. These problems contain the computer model of the thermal energy storage unit with a phase change material filled in plates. In the first problem a different configurations of the plates were considered with constraints to maximal and minimal number of the plates in a storage unit. It was confirmed that the best feasible solution was also a global maximum. In the second problem the thickness of the plates as well as their configurations were unknown parameters to be determined by the optimization. The number of plates was bounded by a total mass of a phase change material available to fill into plates. Obtained results are discussed and presented in graphs and tables for easier comparison of obtained values.

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Used symbols and abbreviations

Symbol	Unit	Veličina
A_c	m^2	cross-sectional area
Bi	-	Biot number
c	J kg^{-1} K^{-1}	specific heat for incompressible substances
c_{eff}	J kg^{-1} K^{-1}	effective specific heat
c_p	J kg^{-1} K^{-1}	specific heat at constant pressure
c_v	J kg^{-1} K^{-1}	specific heat at constant volume
$\dot{E}$	J	energy
E^{tot}	J	total energy
f_s	-	solid phase fraction
Fo	-	Fourier number
$\dot{G}$	J	heat generation rate
H	J	enthalpy
h	W m^{-2} K^{-1})	convective heat transfer coefficient
k	W m^{-1} K^{-1})	thermal conductivity
L	J kg^{-1}	specific latent heat
L_c	m	characteristic length
L_f	J kg^{-1}	specific latent heat of fusion
m	kg	mass
$\dot{m}$	kg s^{-1}	mass flow rate
Nu	-	Nusselt number
P	m	perimeter
Q	J	heat
$\dot{Q}$	W	heat transfer rate
R	K W^2	thermal resistance
Re	-	Reynolds number
t	s	time
T	K	temperature
T_s	K	surface temperature
T_∞	K	ambient fluid temperature
U	J	internal energy
v	m s^{-1}	velocity
V	m^3	volume
$\dot{V}$	m^3 s^{-1}	volumetric flow rate
α	m^2 s^{-1}	thermal diffusivity
ν	m^2 s	kinematic viscosity
μ	N s m^{-2}	dynamic viscosity
ρ	kg m^{-3}	density