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COMPUTATIONAL HEAT TRANSFER WITH PHASE CHANGES IN LATENT HEAT THERMAL ENERGY STORAGE AND STEELMAKING

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COMPUTATIONAL HEAT TRANSFER WITH PHASE CHANGES IN LATENT HEAT THERMAL ENERGY STORAGE AND STEELMAKING

VÝPOČTOVÉ MODELOVÁNÍ PŘENOSU TEPLA S FÁZOVÝMI PŘEMĚNAMI V ÚLOHÁCH AKUMULACE TEPLA A VÝROBY OCELI

ZKRÁCENÁ VERZE HABILITAČNÍ PRÁCE

OBOR KONSTRUKČNÍ A PROCESNÍ INŽENÝRSTVÍ

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About the author

Dr Lubomír Klimeš was born on March 20, 1986 in Brno, the Czech Republic. He received the BSc degree in the branch of Mathematical Engineering from Brno University of Technology in 2008. In the follow-up double diploma study, he defended his master thesis entitled *Stochastic programming algorithms* and he received the double diploma MSc degrees from Brno University of Technology and from Università degli Studi dell'Aquila, Italy, in 2010. He continued with a doctoral study at Energy Institute, Brno University of Technology, and he defended his doctoral thesis *Optimization of secondary cooling parameters of continuous steel casting* in 2014 and received the PhD degree in the branch of Design and Process Engineering.

Since 2014, Dr Klimeš has been working in a full-time position at Energy Institute at Faculty of Mechanical Engineering, Brno University of Technology. He is an assistant professor focusing on education and teaching as a member of academic staff, and he is also a researcher participating in research projects. As for his teaching activities, he teaches tutorials in thermodynamics and heat transfer (the course entitled *Thermomechanics*) and a seminar of applied thermodynamics (the course entitled *Seminar of applied thermomechanics*). Dr Klimeš has also been acting as a supervisor of bachelor and master students, and currently he is a co-supervisor of two PhD students.

The research interests of Dr Klimeš mainly involve computational heat transfer with phase change and related applications. These particularly include efficient utilisation of energy resources by means of latent heat thermal energy storage, and optimal control and optimisation of continuous steel casting with the use of computer models. Dr Klimeš has participated in a number of research projects on these topics funded from various sources, e.g. projects *Sustainable process integration laboratory (SPIL)* and *Computer simulations for low-emission energy* (funded from the ERDF), projects *A coupled real-time thermo-mechanical solidification model of steel for crack prediction*, *Hysteresis of the temperature–enthalpy curve during partial phase change of latent heat storage materials* and *An adaptive front tracking method for parallel computing of phase change problems* (funded by the Czech Science Foundation), or projects *Advanced nature-inspired methods optimisation methods and their HPC implementation for solution of real problems* and *Phase change materials for increased energy efficiency of air-based solar thermal systems in buildings* (COST-Action projects). He published 22 papers in journals having impact factor, he received 228 citations and his h-index is 8 (according to data in Scopus on Aug 6, 2019). Dr Klimeš has also cooperated with industry, e.g. with Železiarny Podbrezová steelworks, Slovakia (development and use of a dynamic solidification model for continuous steel casting) and with Doosan Škoda Plzeň, the Czech Republic (a simulation model for optimal start-up and shut-down of steam turbines and a computer model of air-cooled condensers).

As for international experience and cooperation, Dr Klimeš studied two semesters of his master study at Università degli Studi dell'Aquila in L'Aquila, Italy (2008–2009). In 2014, he undertook a two-week short-term research stay at Universidad de Zaragoza in Zaragoza, Spain. And for 6 months in 2019, Dr Klimeš was a visiting researcher at Concordia University in Montreal, Canada, and working on topics related to thermal energy storage.

1 Introduction

In recent years, a great attention of researchers as well as politicians has been devoted to sustainable utilisation of energy, water, and other natural resources, and to minimisation of negative impacts of human activities to the natural environment. This includes the transition from fossil fuels to renewable resources of energy, improvement of energy efficiency, minimisation of water footprint as well as the reduction of production of emissions and greenhouse gases , which mainly contribute to global warming. It was well reported that global warming represents a serious threat to the natural environment and can result in a wide range of harsh environmental impacts [2].

As for the utilisation of renewable energy resources, solar energy represents a renewable energy resource with a great opportunity for utilisation. Basically, there are two main forms of energy, into which the solar radiation can be converted: heat and electricity. The energy conversion of solar energy (radiation) to heat is easier than in case of electricity and there are many well-established applications available for this purpose. They include, for instance, solar heaters of air and water, which allow for solar heating of air and water and their further use for space heating and other utilisation in buildings. The second way—the energy conversion of solar energy to electricity—requires the use of solar cells, which convert solar radiation directly to electricity. Another example of the solar energy utilisation combining both heat and electricity together is the solar concentrated power generation (solar–thermal power plants). In the solar–thermal power plant, heliostats are used to concentrate solar radiation to a receiver. The receiver converts solar radiation to heat, which is used as a heat source in a thermodynamic cycle for electricity generation.

However, the main drawback of solar energy is that the energy demand usually does not meet the energy supply as these two are shifted in time. Moreover, solar energy is not evenly distributed over a day, nor over a year. Simply speaking, for instance, solar radiation is well available during a sunny day, but at that time requirements for space heating are rather low. Instead, solar energy would be employed much more efficiently after the sunset when solar radiation is no more available but when a need for space heating arises. This implies that ways for thermal energy storage are a crucial issue for an efficient utilisation of solar energy.

There exist several approaches for thermal energy storage. Latent heat thermal energy storage (LHTES) and the use of phase change materials (PCMs) seem to be a promising way for mitigation of energy consumption applicable in buildings. It is well reported that buildings are responsible for about 40% of the total world energy consumption [18]. Moreover, heating, ventilating and air conditioning systems account for about 60% of energy consumed in buildings [28]. The principle of LHTES and PCMs is to employ the heat of fusion accompanying the phase change for the increase of the thermal storage capacity. There are many applications of LHTES and PCMs integrated in building structures. Examples include solar air heaters, heat storage units (for energy storage, energy peak shaving, and for reduction of mismatch between the energy demand and energy supply mentioned above), and building structures with an integrated PCM, which allow, e.g., for an improved thermal comfort, for preventing a room from overheating and temperature fluctuations, and for the increase of thermal inertia of lightweight buildings. The efficient utilisation, design, and optimisation of such systems cannot be accomplished without the use of computer simulations. The computer models of these systems pertain to computational heat transfer with phase changes. Though great knowledge in this area is available, there is still an extensive research of such systems, which is mostly aimed at the transition of ideas and prototypes into practice.

As already mentioned at the beginning of this chapter, another current concern of researchers as well as politicians is the efficient use of natural resources, minimisation of emissions, and the reduction of the water consumption. Steel industry including ironmaking and steelmaking is an important industrial sector, which accounts for a huge consumption of energy, water, and natural resources—especially iron ores. It is reported that about 20.3 GJ of energy is required in all processes involved in the production of one tonne of steel [86]. Moreover, about 4 m^3 of fresh water are consumed per one tonne of the crude steel output [82]. Considering the recent total world apparent steel production (i.e. finished steel products) of about 1,600 million tonnes [86], the steel industry represents a substantial consumer of vast amounts of energy and water. Therefore, even a reduction in the magnitude of 0.1% of the consumption of resources allows for significant savings.

At the moment, the steelmaking method of continuous steel casting is used for more than 98% of the total world steel production. The proper setup, the determination of casting parameters, and optimisation of the casting process with the aim to minimise quality issues (e.g. crack formation, centre-line segregation), the energy consumption, and the water use cannot be accomplished without the use of computer simulations. As in case of LHTES systems with PCMs, computer modelling of continuous steel casting pertains to computational heat transfer with phase changes. In fact, many issues, approaches, and conclusions are common and well applicable for computer modelling of LHTES systems with PCMs as well as for modelling of continuous steel casting, though these areas may seem to be rather distinct at the first glance.

The aim of the thesis is to provide an insight into the current development in computer modelling of LHTES systems with PCMs as well as in computer modelling of continuous steel casting, and to demonstrate the author's contribution to these research fields. The thesis consists of two rather comprehensive chapters. Chapter 2 is devoted to LHTES systems, PCMs, and their computer modelling and utilisation in solar air systems with heat storage units and in building structures integrating PCMs. Chapter 3 is focused on continuous steel casting, its computer modelling, and the use of models for the casting process control and optimisation. Each of these two chapters first provides an overview of the current development in the field, which is followed by briefly commented journal papers co-authored by the author of the thesis demonstrating his contribution to the field. The presented overview in each chapter serves as a wider insight to the current state and development in the field, and it is not aimed at the assessment of the author's published papers with related works of other investigators. This is presented in each paper individually (mainly in the introduction section and/or in the section providing a review on the topic) with identification of the contribution to the field as well as with the specified research gap and novelty covered by the paper.

Overall, the thesis contains ten journal papers co-authored by the author of the thesis. Each presented paper has been published in a peer-review journal having an impact factor according to Web of Science. Six papers are included in Chapter 2, while four papers in Chapter 3. Among the included ten papers, six papers are contained in the first quartile of mostly energy-related areas according to the Journal Citation Reports (JCR) and the journal impact factor (JIF) in Web of Science. Three papers are even included in the first decile, which contains top 10% journals in each category. The highest impact factor of the included papers is 9.18, and the sum of received citations to the included papers is 123 according to the Google Scholar.

2 Phase change modelling and utilisation of systems for latent heat thermal energy storage

Energy represents a key ingredient in the current technological and economic development of the society. As reported by many investigators, energy resources of non-renewable energy have become more and more limited. Together with the consideration of global warming, the trend and focus have moved to sustainable and renewable energy resources. However, in the utilisation of renewable energy resources the crucial problem is that the energy demand very often does not meet the energy supply in the time scale. This is especially the case of solar and wind renewable energy. In such instances, mechanisms and technologies are needed to shift the energy supply and make it available in periods with the energy demand. Since the storage of higher forms of energy such as the electricity is rather difficult, the thermal energy storage with heat as the lowest form of energy is often utilised as heat is relatively easy to store. Moreover, heat is very often the required final form of energy supplied to customers, which makes the thermal energy a suitable way for energy storage.

2.1 Thermal energy storage

Thermal energy storage (TES) is a way how to store energy in the form of heat—thermal energy. There are basically three approaches applicable for the TES [9]: the sensible heat TES, the latent heat TES, and the thermochemical TES, but the most TES systems employ the first two approaches: the sensible and latent heat TES. As for the sensible heat TES, heat can be accumulated and stored in a material by means of increasing its temperature in the form of sensible heat. The sensibility here means that any change in the amount of heat accumulated to or released from the material causes a direct change of its temperature. On the other hand, the latent heat TES (LHTES) employs a phase change (including both changes with and without the change of the state) and its latent heat to store thermal energy. Examples of phase changes include the melting, solidification, boiling, condensation, sublimation, and desublimation. The term latent heat is frequently used, however it makes sense only in case of materials such as pure chemical elements (such as iron), which change the phase at a constant temperature. In such case, heat accompanying the phase change is indeed latent meaning "hidden" as it cannot be observed as a change of the temperature. In the majority of practical applications of TES, complex substances, composite materials, mixtures, and alloys are utilised rather than pure chemical elements. In such cases, the phase change does not occur isothermally but in a certain temperature interval (cf. iron and steel). Therefore, in these instances it is more precise to refer heat required for the phase change as the heat of fusion.

2.2 Latent heat thermal energy storage

Latent heat thermal energy storage (LHTES) represents an efficient way how to store energy in the form of heat—thermal energy. In contrast to the sensible heat, the latent heat (heat of fusion) allows for the accumulation and release of a relatively large amount of heat in a narrow temperature interval, or even at a constant temperature. In other words, heat can be stored to a suitable material without increasing its temperature very much; instead of raising the temperature, the change of phase accompanied by the heat of fusion is utilised as a heat reservoir. This allows for a significantly larger thermal capacity of LHTES systems when considering the latent heat and the sensible heat TES in a fixed temperature interval. Due to these reasons, the attention of researchers and investigators has focused on the utilisation of LHTES for an efficient use of energy resources in the last 15–20 years. As already mentioned, this has particularly been the case of renewable energy resources such as solar energy, where the LHTES technique can be used to balance between the energy demand and the energy supply.

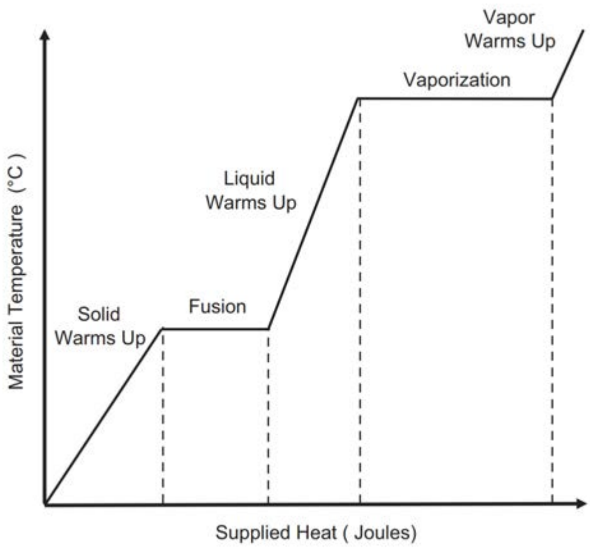


Figure 2.1: Dependence of the temperature on the heat transferred to a material [9]

Figure 2.1 demonstrates the influence of sensible heat and latent heat supplied to a storage material undergoing two phase changes: melting (fusion) of the solid to the liquid, and vaporisation of the liquid to the gas. The material, for which the plot in Figure 2.1 is shown, undergoes the phase changes isothermally as a pure chemical element. In case of a complex substance (a mixture), some raise of the temperature would be visible during the phase change processes. However, gradients of the phase change lines would be much smaller than gradients for sensible heat TES (all remaining lines in Figure 2.1). Applications of both the solid-liquid and liquid-gas phase changes can be found in the literature. However, the majority of LHTES systems utilises the solid-liquid transformation for its more suitable properties and behaviour mentioned e.g. in [20].

As for the quantification of heat stored in the latent heat TES material undergoing the isothermal phase change from the solid state to the liquid state, the amount of heat transferred to the material in the temperature range between T_i and T_f can be determined as [9]

$$Q = \int_{T_i}^{T_m} mc_p \,\mathrm{d}T + m\Delta H_m + \int_{T_m}^{T_f} mc_p \,\mathrm{d}T \tag{2.1}$$

where T_m is the phase change temperature and ΔH_m is the latent heat of the solid-liquid phase change (the heat of fusion). As for paraffins (organic phase change materials discussed in the following section), which are mostly considered in LHTES applications presented in this thesis, their heat of fusion is about 200 kJ/kg [23]. Thus, with the assumption of the specific heat of 2 kJ/kg·K [56] their heat storage capacity in the temperature range of 20 K including and excluding the phase change is about 240 kJ/kg and 40 kJ/kg, respectively. Considering two typical sensible heat storage media–pebbles (stone) and water–their specific heat is about 0.9 kJ/kg·K and 4.2 kJ/kg·K, respectively [13]. For the identical temperature range of 20 K, the TES capacity for pebbles and water is 18 kJ/kg and 84 kJ/kg, respectively. From this point of view, it is obvious that the heat of fusion and the phase change play crucial roles for the thermal capacity available for TES. In other words, the LHTES allows for a higher heat storage density than in case of the sensible TES. Therefore, a smaller amount of the heat storage material is needed in case of the LHTES system, which implies lower requirements on space and its easier integration.

There are numerous designs and applications of LHTES and some of them are discussed in more detail in Section 2.4. In a general view, these systems for LHTES can be considered as heat exchangers: devices for heat transfer between a heat storage material changing the phase and a suitable heat transfer fluid. Such heat exchangers can be of different designs and concepts: including traditional closed-system heat exchangers [10] (e.g the shell with a heat storage material inside and a heat transfer fluid flowing through the shell) as well as open systems such as wall panels with LHTES installed in the room and the ambient air interacting with the panels [34].

2.3 Phase change materials

As explained in the previous section, the LHTES allows for a higher thermal capacity than in case of the sensible TES when considering the identical temperature range in both cases. Due to this reason, the LHTES has attracted a great attention of investigators and developers in the two last decades, which is confirmed by a vast number of original research papers as well as highly cited review papers on related topics, e.g. [1, 8].

LHTES applications are based on the use of phase change materials (PCMs), which are able to change the phase in a desired temperature range [60]. In most cases, the solid-liquid phase change is employed. There is a wide range of PCMs available with various phase change temperatures suitable for low temperature applications (-20 °C to 5 °C), medium temperature applications between 5 °C and 80 °C as well as for high temperature applications above 80 °C. The largest sub-class with medium temperature applications is usually further split into two groups: medium low temperature applications between 5 °C and 40 °C, which typically include heating and cooling in buildings, and medium high temperature applications between 40 °C and 80 °C including solar air and water heating [16].

The PCMs can be classified into three categories according to their chemical composition: organic, inorganic, and eutectic [6]. The organic PCMs represent the majority of the PCMs used in applications operating in the medium low temperature range. Alkanes, often referred to as paraffins or waxes, are the typical and the most frequently utilised organic PCM. The alkanes are organic compounds consisting of carbon and hydrogen atoms according to the formula $CH_3(CH_2)_nCH_3$ with single carbon-carbon bonds only. The phase change temperature of paraffins depends on the number of carbons in the compound: the higher the number of the carbon atoms, the higher the phase change temperature. For example, $C_{12}H_{26}$ has the phase change temperature of about -9 °C, while in case of $C_{44}H_{90}$ it is almost 86 °C [14]. As it is rather difficult to prepare a paraffin consisting of only one alkane, commercially available PCMs usually consist of a mixture of paraffins. This implies that such a paraffin mixture allows for the phase change in a certain temperature range, which is dependent on the compounds and their mass ratios in the mixture.

Besides the alkanes, the class of organic PCMs include other organic materials such as fatty acids, esters, alcohols, and glycols. They have very suitable properties for LHTES applications, however they are about three-times more expensive than paraffins. This makes them minor organic PCMs when considering the number of applications.

As for inorganic PCMs, salt hydrates are a typical representative of inorganic PCMs. They possess a high amount of the heat of fusion as well as a relatively high thermal conductivity (in comparison to paraffins), they are cheap and no-flammable. However, most of them are corrosive to the majority of metals, and they suffer from both supercooling and phase decomposition. Moreover, the salt hydrates degrade in cyclic operation meaning that the heat storage capacity decreases with the increasing number of phase change cycles [6].

Eutectic PCMs are compounds consisting of two or more PCMs. The eutectics form blend crystals when they solidify [2]. According to components in the mixture, the eutectic can be of three types: organic–organic, organic–inorganic, and inorganic–inorganic. The eutectics do not suffer from phase separations and all the components of the mixture change the phase simultaneously.

2.4 Applications of latent heat thermal energy storage

In the last 20 years, a vast number of research papers and studies have been published on the topic of LHTES applications. There are many research and application areas, which make use LHTES and PCMs. As already mentioned in the foregoing sections with the description of types and classification of PCMs, PCMs can be used for applications with very low temperatures such as in cryogenic cooling [74] to very high temperatures such as in concentrated solar power generation [43]. Two application areas of LHTES and PCMs are discussed in more detail in the following paragraphs: solar air heating and cooling systems using thermal storage units, and building structures integrating PCMs. All these applications have been studied with the aim of efficient energy utilisation and/or improvement of thermal comfort in buildings.

2.4.1 Solar air heating and cooling systems with LHTES

Solar air heating and cooling are techniques, which can be used for heating, cooling and conditioning of air in buildings or in other applications [69]. Solar systems employ the renewable solar energy as a source of heat. The integration of the LHTES units with a PCM into the solar air system can benefit in the increase of its thermal performance. In particular for the space heating case, the use of a PCM allows to accumulate and store thermal energy during the day when the solar radiation is available. After the sunset, thermal energy stored in the PCM can subsequently be released and used for space heating [75]. This approach helps to meet the energy supply and demand, which do not occur at the same time. A simple and straightforward utilisation of the solar system for heating is the use of the flat plate solar collector coupled with a heat storage unit as shown in Figure 2.2. The air heated in the solar collector during the day is supplied by the fan to the heat storage unit, where heat is transferred from the air to the PCM, which melts as a consequence of heat transfer into it. The air exiting the storage unit is returned to the ambient environment. When the stored heat is needed, the cold ambient air flows through the heat storage unit and heat transfer occurs in the opposite direction: the PCM solidifies and the released heat is transferred to the air increasing its temperature. The heated air is then supplied to the room. Another design consists of the solar air heater (collector), which directly incorporates the heat storage medium and no separate heat storage unit is needed. A schematic of such design is illustrated in Figure 2.3 [5].

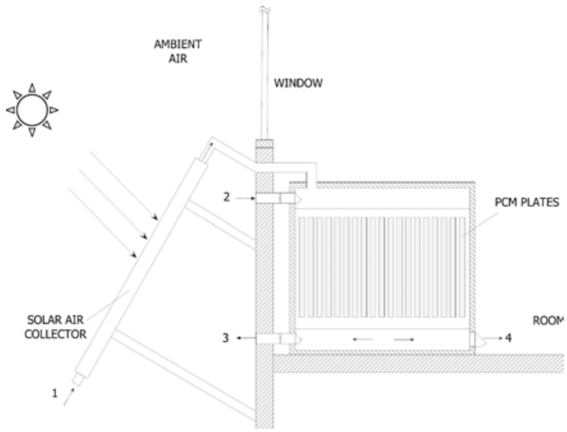


Figure 2.2: Schematic of the solar air system with the solar air collector and the heat storage unit [72]

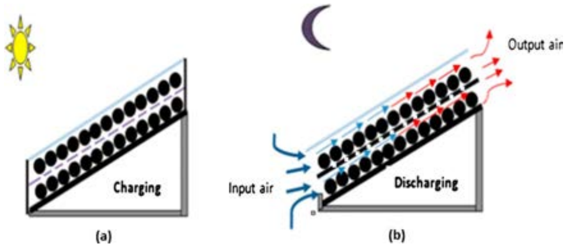


Figure 2.3: Schematic of the solar air heater with an integrated LHTES [5]

A similar principle can be utilised in case of cooling [57]. During the night when the ambient air temperature is lower than the desired room temperature, the ambient air is forced through the storage unit where the PCM solidifies and cold is stored. During the day, the ambient air temperature raising over the desired room temperature can be conditioned by means of the air flow through the storage unit. In this case, the cold stored in the PCM is released to the air, which decreases its temperature (i.e. heat from the air is transferred to the PCM, which causes its melting) [70]. Lin et al. [42] reported on the multi-objective optimisation of the air-PCM heat storage unit for solar air systems. The authors first performed experimental investigations, which were followed by the development of a computer model. A genetic algorithm was coupled with the computer model and an optimisation study was performed. The authors reported that the optimised heat transfer effectiveness can be improved by about 15% with the simultaneous reduction of the charging time by about 1.2 hour.

2.4.2 Air-PCM heat storage units

Heat storage units are technical devices, which are designed to accumulate, store, and consequently release energy in the form of heat. In this section, the attention is focused on storage units, which employ air as the heat transfer fluid. As already explained in the foregoing paragraphs, the heat storage unit is often used as a part of the solar air heating system. However, the heat storage unit can also be used with other sources of energy. A system consisting of the electric heater and the heat storage unit [22] is an example how the LHTES system can be employed for the shift of peak demands of electricity, which are used for heating or cooling in buildings as well as in some industrial applications [65].

Farah et al. [19] reported a study aimed at the investigation of space cooling by means of the air-PCM heat storage unit coupled with the air source heat pump. The storage unit consisted of thin plates made of a PCM as shown in Figure 2.4. The authors developed a 2D computer model of the unit and verified it with the use of experimental data. A sensitivity analysis was carried out with the aim to assess the influence of uncertainties of the phase change temperature and of the inlet air temperature on computational results. It was reported that the uncertainty of these variables has a rather small effect on the electrical energy consumption and the power demand of the cooling system. Further, the authors reported that the use of the thermal storage unit in a proper configuration allowed for the reduction of the annual cooling energy required by the heat pump by about 25%.

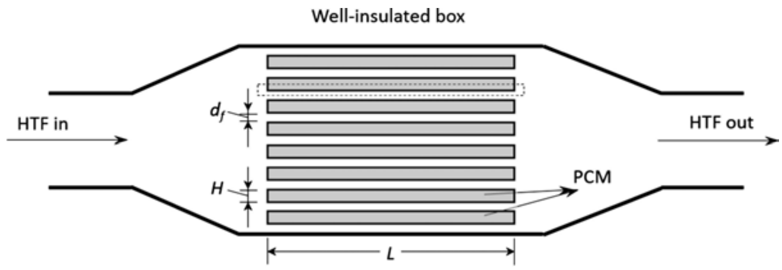


Figure 2.4: Heat storage unit used for space cooling investigated in [19]

Kumirai et al. [40] experimentally investigated an LHTES system consisting of commercially available containers with a PCM for space cooling as shown in Figure 2.5. Three PCMs were considered in the study: two paraffins and salt hydrate with the phase change temperature between 22 °C and 28 °C. The containers were positioned vertically with the gap of 15 mm. An analysis was carried out to investigate the influence of the inlet air temperature and the mass flow rate of the air through the system. It was found that the average thermal efficiency of the system decreased with the increased velocity of the air, and the cooling power increased with the flow rate and with the inlet air temperature. It was further reported that paraffins exhibited a faster and more intensive heat absorption than the considered salt hydrate.

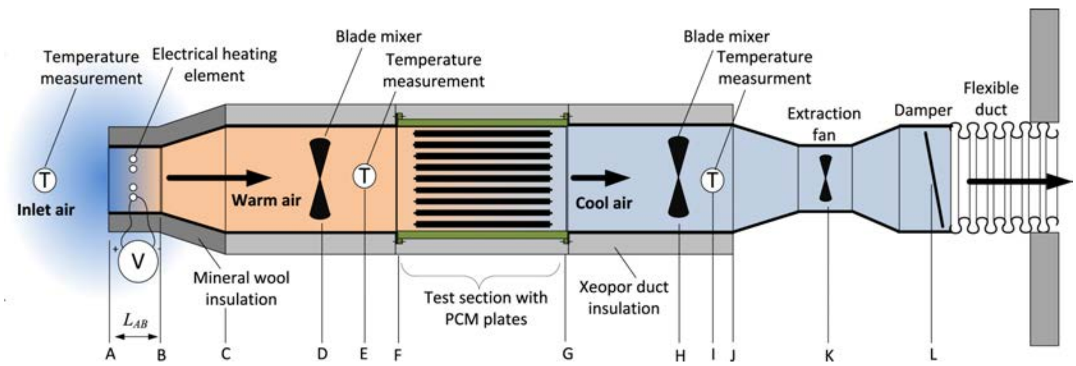


Figure 2.5: The top view of the heat storage system for space cooling analyzed in [40]

Waqas et al. [84] presented a study into the performance of the heat storage unit with a PCM in the form of plates. The computer model of the unit was developed and used for the analysis. The city of Islamabad was considered in the study. It was reported that the performance of the storage unit was maximal for the phase change temperature of about 29 °C in the summer season and for about 21 °C in the winter season. The phase change temperature of 27.5 °C was identified as an optimum for the all-the-year operation of the unit. Moreover, it was concluded that the decrease of the heating capacity was not as sharp as the decrease of the cooling capacity. If, for instance, a PCM with the phase change temperature of 29 °C is used instead of 27.5 °C, the cooling capacity is increased by 15%, while the heating capacity is decreased only by 3%.

2.4.3 Building structures integrating PCMs

The use of PCMs in building structures represents another frequent application of the LHTES. The main aim of the integration of PCMs in building structures is the improvement of thermal conditions, thermal comfort and environment in buildings. The integration of PCMs enables, for instance, the increase of thermal inertia of lightweight buildings, for the stabilisation of air temperature fluctuations, prevents overheating, and allows for the reduction of energy consumption needed for space heating and cooling. Dominantly, a vast number of research works can be found in relation to the integration of PCMs into walls and vertical building structures. However, the use of PCMs in horizontal building structures such as in floors and ceilings has also been widely reported. In the following text, several recent examples of achievements in the utilisation and integration of PCMs in vertical building structures are given and briefly commented to illustrate current research interests and objectives.

De Gracia [12] presented a novel concept based on the dynamic use of PCMs in building envelopes as shown in Figure 2.6. The proposed solution allows to set up the position of the PCM layer inside the building envelope with respect to the insulation layer. The author provided a proof of concept for this technical solution based on computer simulations. The phase change temperature and the control of the position of the layer with the PCM were optimised using a particle swarm optimisation method. The simulation results indicated that the dynamic adjustment of the PCM layer significantly facilitates the solidification of the PCM, which allows for the use of a PCM with a lower phase change temperature.

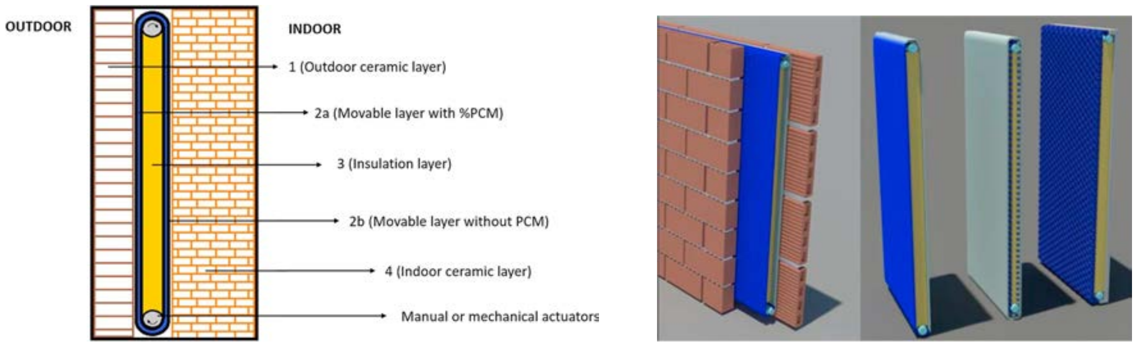


Figure 2.6: The schematic of the wall with the adjustable PCM layer investigated in [12]

Mi et al. [51] analysed the influence of a PCM layer in the building envelope (shown in Figure 2.7) on energy consumption of a multistory office building. The computer model in EnergyPlus and a whole-year simulation were utilised and five locations with different climate conditions were considered in the study. The authors reported that energy savings are significant in cases with cold climate regions as well as in regions with hot summer and cold winter. It was already reported that though the use of PCM in wall structures is economically attractive in some locations, there are also locations in which the investment to the PCM cannot be recovered, and thus is not economically viable. Therefore, each installation has to be considered separately and properly addressed taking into account the whole-year conditions. Zwanzig et al. [87] investigated the potential of energy savings by means of the integration of PCM into the building envelope. The authors created a computational model of the wall, which was coupled with with meteorological data applied for exterior boundary conditions. It was concluded that the thermal performance of the PCM highly depends

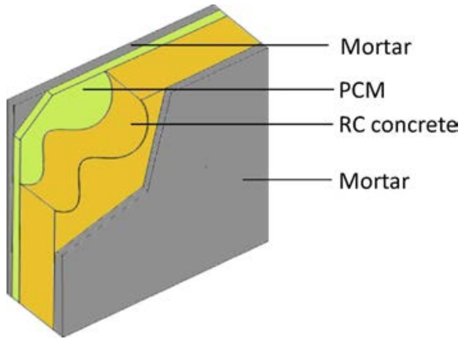


Figure 2.7: The wallboard with a PCM investigated in [51]

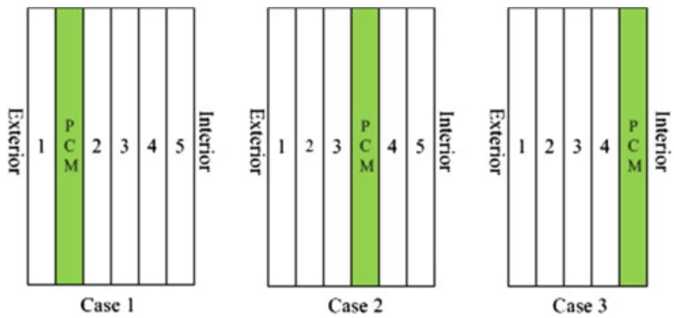


Figure 2.8: Optimal location of the PCM layer analysed in [87]

on weather conditions, which means that a suitable PCM has to be selected according to a particular climate region. The authors also analysed different locations of the PCM layer in the wallboard as shown in Figure 2.8. It was demonstrated that the optimal location of the PCM layer is a function of the thermal resistance between the PCM layer and the exterior boundary conditions.

2.5 Modelling of LHTES systems with PCMs

In general, computer modelling of systems for LHTES and including PCMs pertains to computational heat transfer with phase changes. In contrast to other research areas including the solution of heat transfer problems with phase changes, simpler and straightforward numerical methods and approaches are often used in the majority of models for LHTES in building applications rather than complicated, comprehensive, and computationally demanding techniques. This is also the case of solar air heating and cooling systems, thermal storage units consisting of commercially available plates with PCMs, and building structures with integrated PCMs discussed in this thesis. There are probably several reasons for it; the most important ones are that (1) in many cases the heat transfer problem can be simplified and considered as a 1D or 2D problem, (2) natural convection has often minor effects and can be neglected, and (3) models need to be computationally effective as they are frequently used for simulations of long-term periods, such as several weeks or months, or even a whole year. However, advanced methods such as CFD should be used in cases in which the geometry is rather complex and/or multiphysical phenomena such as heat conduction–convection with fluid flow have to be taken into consideration [3].

Agyenim et al. [1] thoroughly reviewed heat transfer and phase change formulations for LHTES systems. The authors concluded that the enthalpy method has been the most frequently utilised approach used for taking into account the phase change and the evolution of the heat of fusion. It was also pointed out that though only pure conduction was previously solely taken into consideration, current models also account for convection in the melt in cases where convection represents a non-negligible heat transfer mechanism. The authors reported that in case of modelling of PCMs and LHTES systems, the analysis is complex and includes the solid–liquid moving boundary problem. The position of the boundary (the interface between the phases) is unknown and needs to be determined as a part of the solution.

General formulation of a phase change problem. In case of the two-phase heat transfer problem driven by heat conduction, its solution consists of the time-dependent temperature distribution and of the time-dependent phase change location for the phase change problem with a moving interface [4]. In case of PCMs, the solid-liquid phase change is dominantly utilised. The temperature distribution of the solid phase is governed by the heat transfer equation

$$\varrho_{\mathrm{s}} c_{p,\mathrm{s}} \frac{\partial T_{\mathrm{s}}}{\partial t} = \nabla \cdot (k_{\mathrm{s}} \nabla T_{\mathrm{s}}) \tag{2.2}$$

where ϱ is the density, c_p is the heat capacity, T denotes the temperature distribution, t is time, and k stands for the thermal conductivity. The subscript s indicates that the quantities are related to the solid phase. Similarly, for the liquid phase the governing equation is

$$\varrho_{\ell} c_{p,\ell} \frac{\partial T_{\ell}}{\partial t} = \nabla \cdot (k_{\ell} \nabla T_{\ell}) \tag{2.3}$$

which is the identical equation as in case of Eq. (2.2), only the temperature and the thermophysical properties of the liquid phase are used as indicated by the subscript ℓ. The balance on the interface between the phases as well as the behaviour of the interface (its movement and shape) are governed by the Stefan condition [4, 79]

$$k_{\mathrm{s}} \frac{\partial T_{\mathrm{s}}}{\partial n} - k_{\ell} \frac{\partial T_{\ell}}{\partial n} = \varrho \Delta H_{\mathrm{m}} \frac{\mathrm{d}s}{\mathrm{d}t} = \varrho \Delta H_{\mathrm{m}} v_n \tag{2.4}$$

where ΔH_{m} is the amount of the latent heat, s is the location of the interface, and v_n is the normal velocity of the interface. In general, the solution of the phase change problem requires the simultaneous solution of all three aforementioned equations (2.2), (2.3), and (2.4). This is, for example, the case of the front tracking method, which is discussed in detail in a paper [35] in Section 2.6. However, the widely used enthalpy method and the effective heat capacity method overcome this issue and they reduce Eqs. (2.2)–(2.4) into a single governing equation as explained below.

Enthalpy method. The method is based on the use of the enthalpy—a thermodynamically defined function, which allows for the inclusion of both the sensible heat and the heat of fusion. The enthalpy H can be defined [73] as a function of the temperature T according to

$$H(T) = \int_{T_{\mathrm{ref}}}^{T} \left(\varrho c_p - \varrho \Delta H_{\mathrm{m}} \frac{\partial f_{\mathrm{s}}}{\partial \vartheta} \right) \mathrm{d}\vartheta \tag{2.5}$$

where ϱ is the density, c_p is the heat capacity, f_{s} is the solid fraction, and T_{ref} is a reference temperature. The substitution of Eq. (2.5) to the heat transfer equations (2.2) and (2.3) requires no more consideration of Eq.(2.4) as the evolution of the heat of fusion is now incorporated in the enthalpy and in Eq. (2.5), and the governing enthalpy-formulated heat transfer equation [73] reads

$$\frac{\partial H}{\partial t} = \nabla \cdot (k \nabla T). \tag{2.6}$$

As can be observed there are no subscripts s and ℓ in Eq. (2.6). It means that Eq. (2.6) serves as the governing equation for both the phases, which are not explicitly separated. However, it is worth pointing out that the thermal conductivity k is in fact a function of the local temperature.

Effective heat capacity method. Similarly as in case of the enthalpy method, the effective heat capacity method uses the heat capacity c_p, often referred to as the specific heat, for the inclusion of the latent heat. The effective heat capacity then accounts for both the sensible heat and the heat of fusion, typically as a function of the local temperature $c_{\mathrm{eff}}(T)$. The effective heat capacity is related to the enthalpy as [71]

$$c_{\mathrm{eff}} = \frac{1}{\varrho}\frac{\partial H}{\partial T} = c_p - \Delta H_{\mathrm{m}}\frac{\partial f_{\mathrm{s}}}{\partial T}. \tag{2.7}$$

Further, as in case of the enthalpy method, the Stefan condition given in Eq. (2.4) is transformed into Eq. (2.7) and the substitution of Eq. (2.7) into the heat transfer equations (2.2) and (2.3) leads to the governing effective-heat-capacity-formulated heat transfer equation

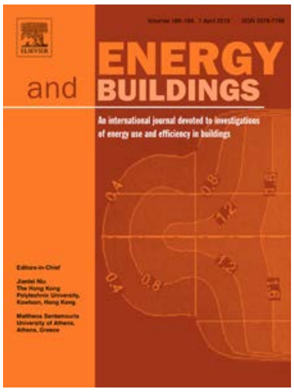
$$\varrho c_{\mathrm{eff}}\frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T). \tag{2.8}$$

Similarly as in case of the enthalpy method, Eq. (2.8) accounts for both the phases, and ϱ, c_{eff}, and k are functions of the local temperature.

The enthalpy method and the effective heat capacity method with their governing equations (2.6) and (2.8), respectively, represent the most frequently adopted methods for computer simulations of LHTES systems with PCMs. The reason for this is that both these methods are relatively simple, straightforwardly implementable and computationally efficient. It is reported that the enthalpy method offers a slightly better stability and a higher accuracy than in case of the effective heat capacity method, and the enthalpy approach does not require the use of additional techniques for the fulfilment of the energy conservation since the enthalpy method is known to be self-conservative [44, 66]. On the other hand, the enthalpy method requires a two-stage and usually less efficient solution as Eq. (2.6) contains two unknown variables H and T, which need to be sequentially solved in each time iteration. In case of the effective heat capacity method, the temperature T in Eq. (2.8) is the only unknown variable, which makes the method more straightforward.

2.6 Author's contribution to the development of computer modelling and utilisation of systems for latent heat thermal energy storage

Six journal papers co-authored by the author of the thesis and published in peer-review journals having the impact factor in Web of Science are included in the thesis in order to demonstrate the author's contribution to the field of computer modelling and utilisation of systems for latent heat thermal energy storage. The included journal papers are:



[10] Charvát P, Klimeš L, Ostrý M. 2014. Numerical and experimental investigation of a PCM-based thermal storage unit for solar air systems. *Energy and Buildings* **68**: 488–497.

Author's contribution: 45%.

Metrics: $\mathrm{IF}_{2014} = 2.88$. $\mathrm{CiteScore}_{2014} = 4.21$. Citations: 77 (G Scholar).

Ranking: 2×Q1 (2×D1 as well)[a] and Q2 in JCR 2014 WoS.

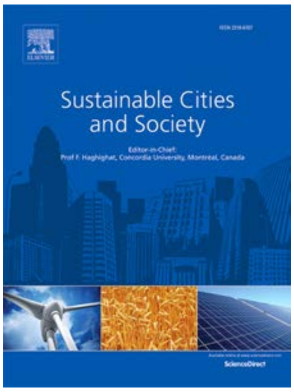
[a] D1 = the first decile = top 10% journals

[35] Klimeš L, Mauder T, Charvát P, Štětina J. 2018. Front tracking in modelling of latent heat thermal energy storage: Assessment of accuracy and efficiency, benchmarking and GPU-based acceleration. *Energy* **155**: 297–311.

Author's contribution: 70%.

Metrics: IF$_{2017}$ = 4.97. CiteScore$_{2017}$ = 5.60. Citations: 2 (G Scholar).

Ranking: 2×Q1 (1×D1 as well) in JCR 2017 WoS.



[72] Stritih U, Charvát P, Koželj R, Klimeš L, Osterman E, Ostrý M, Butala V. 2018. PCM thermal energy storage in solar heating of ventilation air—Experimental and numerical investigations. *Sustainable Cities and Society* **37**: 104–115.

Author's contribution: 45% (considering authors from the Brno University of Technology only).

Metrics: IF$_{2017}$ = 3.07. CiteScore$_{2017}$ = 3.55. Citations: 11 (G Scholar).

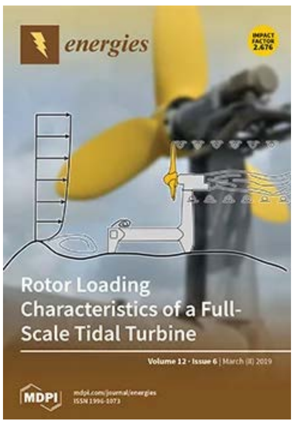
Ranking: Q1 and 2×Q2 in JCR 2017 WoS.

[34] Klimeš L, Charvát P, Ostrý M. 2019. Thermally activated wall panels with microencapsulated PCM: comparison of 2D and 3D models. *Journal of Building Performance Simulation* **12** (4): 404–419.

Author's contribution: 48%.

Metrics: IF$_{2017}$ = 2.60. CiteScore$_{2017}$ = 2.20. Citations: 0.

Ranking: Q1 in JCR 2017 WoS.

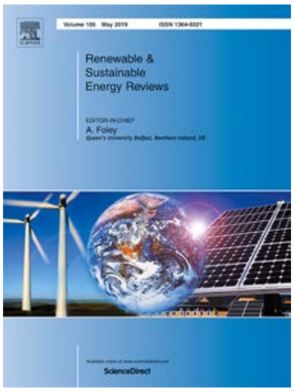


[11] Charvát P, Klimeš L, Zálešák M. 2019. Utilization of an air-PCM heat exchanger in passive cooling of buildings: A simulation study on the energy saving potential in different European climates. *Energies* **12** (6): article 1133.

Author's contribution: 30%.

Metrics: IF$_{2}$017 = 2.68. CiteScore$_{2017}$ = 3.15. Citations: 0.

Ranking: Q2 JCR 2017 WoS.



[62] Pospíšil J, Charvát P, Arsenyeva O, Klimeš L, Špiláček M, Klemeš JJ. 2019. Energy demand of liquefaction and regasification of natural gas and the potential of LNG for operative thermal energy storage. *Renewable and Sustainable Energy Reviews* **99**: 1–15.

Author's contribution: 20% (considering authors from the Brno University of Technology only).

Metrics: $\mathrm{IF}_{2017} = 9.18$. $\mathrm{CiteScore}_{2017} = 10.54$. Citations: 5 (G Scholar).

Ranking: 2×Q1 (2×D1 as well) in JCR 2017 WoS.

Charvát et al. [10]: Numerical and experimental investigation of a PCM-based thermal storage unit for solar air systems

The paper [10] was concerned with the numerical and experimental investigation of a PCM-based thermal storage unit, which was designed for the use in solar air systems. The heat storage unit consisted of 100 aluminium panels (CSM panels) filled with the commercially available PCM Rubitherm RT42. The purpose of the unit was space heating and the unit was designed to operate in two phases. In the charging phase during the day when the solar radiation is available, the hot air (e.g. supplied by a solar collector) is used to charge the PCM: heat is transferred from the air to the PCM, which melts and accumulates heat in the form of the sensible heat as well as of the latent heat of phase change (the heat of fusion). In the discharging phase when heat is needed and solar radiation is no more available (during the evening or the night), the cold air from the ambient environment is used to discharge the PCM in the CSM panels: heat is transferred from the PCM to the cold air, which causes the increase of its temperature. As a consequence of heat withdrawal from the CSM panels, the PCM solidifies and releases the heat of fusion accumulated in the charging period. The heated air is then delivered to the room for its space heating.

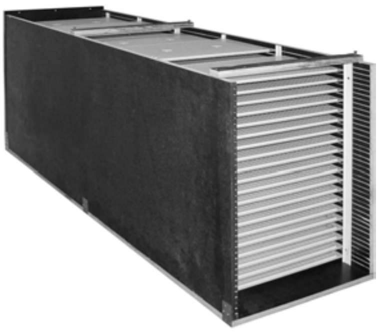


Figure 2.9: Photograph of the experimental unit without front and top walls revealing CSM panels [10]

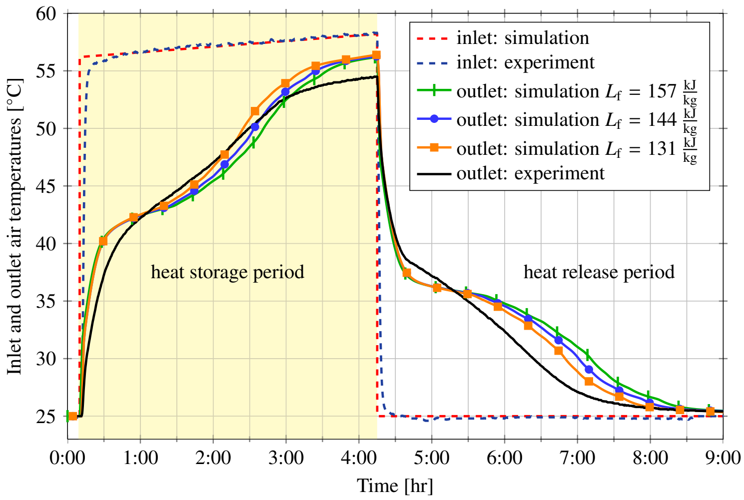


Figure 2.10: Comparison of experimental and simulation results [10]

Both numerical and experimental investigations were performed and discussed in [10]. As for experimental investigations, the unit shown in Figure 2.9 was built and tested in a lab. As a source of heat, an electric heater coupled with the fan was used. Experimental data acquired in the unit testing were consequently used for the validation of the computer model. As for the computer model of the heat storage unit, a standalone model was first developed in MATLAB. After its testing, debugging, and validation, the model was re-implemented to the form of a so-called TRNSYS Type (a DLL library), which is suitable for the use in the TRNSYS simulation tool. The computer model was designed as a quasi 2D model (1D heat transfer was solved in the direction of the thickness of the CSM panels) and the effective heat capacity method was adopted for modelling of the phase change. The model was validated by means of acquired experimental data as shown in Figure 2.10. Once the model was validated, some case studies were performed in order to investigate operational parameters, setup, and thermal behaviour of the heat storage unit. The model was further used for optimal design of the thermal storage unit and the thermal performance was investigated.

Klimeš et al. [35]: Front tracking in modelling of latent heat thermal energy storage: Assessment of accuracy and efficiency, benchmarking and GPU-based acceleration

The study [35] was aimed at the assessment of computer methods for phase change modelling applicable for LHTES. Two kinds of methods were taken into consideration: interface capturing methods and interface tracking methods. As for methods based on interface capturing, the well known enthalpy method, the apparent heat capacity (frequently also referred to as the effective heat capacity method), and the temperature recovery method were incorporated into the study. Those interface capturing methods have dominantly been applied in computational heat transfer with phase changes as these methods are relatively simple and straightforward when considering their underlying principle and implementation. Such methods, however, primarily aim at the determination of the temperature distribution, and the location of the interface separating the phases is somehow determined from the temperature distribution, usually with the use of linear interpolation between nodes identified as nodes having distinct phases. On the other hand, interface tracking methods are proposed for the opposite strategy: first the interface location (the so-called front) and phase domains are accurately determined from the physical balance on the front, and the temperature distribution is consequently determined in the second step. The front tracking methods are reported to have a better accuracy than in case of the interface capturing methods.

The comparison of the interface capturing methods with the front tracking method was performed. The assessment was carried out in terms of the computational accuracy and efficiency. The two Stefan two-phase problems in the semi-infinite 1D domains were used for the assessment of accuracy as analytic (exact) solutions for these problems exist. Figure 2.11 shows the comparison of the computational accuracy in terms of the temperature error in dependence on the spatial coordinate, and in terms of the front location error in dependence on time, respectively. The analysis of the results revealed that the front tracking method allows for a superior computational accuracy when compared to other interface capturing methods. However, the higher computational accuracy of the front tracking method is paid by its lower computational efficiency—the front tracking method was the slowest one when compared with interface capturing methods. Moreover, the implementation and coding of the front tracking method are substantially more challenging than in case of interface capturing methods. Due to the lower computational efficiency, the GPU-acceleration of the front tracking method, which was previously successfully proposed and applied by the author in [38], was utilised to enhance the computational performance.

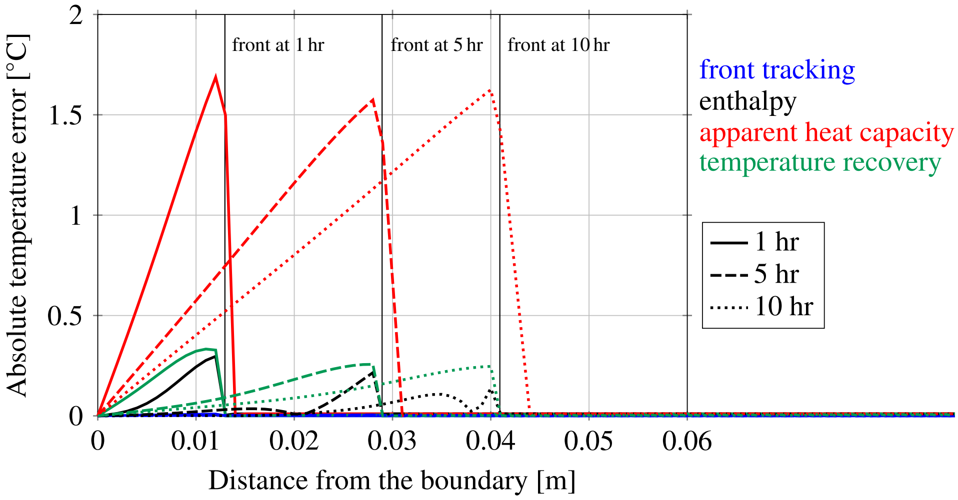


Figure 2.11: Assessment of the computational accuracy: absolute temperature errors as functions of the spatial distribution for the one-phase Stefan melting problem [35]

Stritih et al. [72]: PCM thermal energy storage in solar heating of ventilation air—Experimental and numerical investigations

The paper [72] was aimed at the investigation of the latent heat thermal storage unit for solar heating of ventilation air. The article represents a result of the research cooperation between research teams from the Brno University of Technology and from the University of Ljubljana in Slovenia, which was established in Annex 31 "Energy Storage with Energy Efficient Buildings and Districts: Optimisation and Automation" of the International Energy Agency. The study involved the investigation of the air-PCM storage unit with a similar design to the unit presented in [10]. Experiments as well as computer simulations were performed to assess the applicability of the air-PCM storage unit. The unit consisted of CSM panels filled with the PCM Rubitherm RT 22 HC and the unit was coupled with the solar collector.

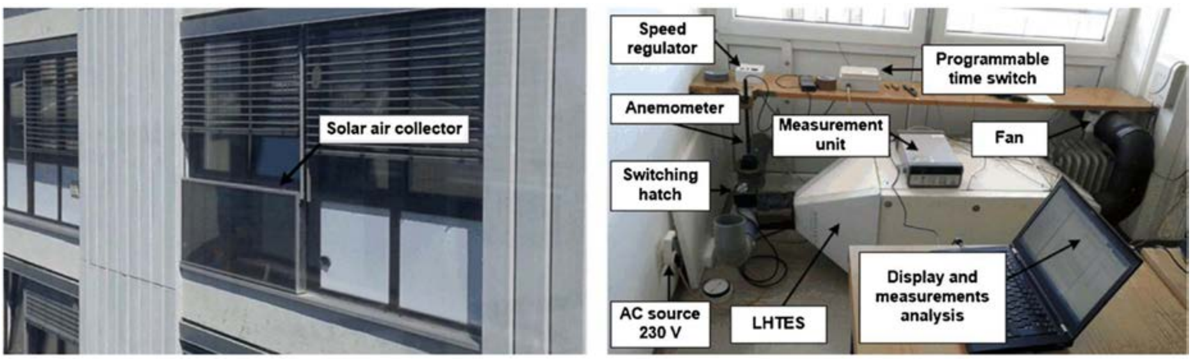


Figure 2.12: Experimental setup of the system with the solar air collector (left) and the heat storage unit (right) [72]

Figure 2.12 shows the solar collector mounted on the exterior wall of a building (left) and the heat storage unit consisting of CSM panels filled with the PCM (right). The system was installed at the Faculty of Mechanical Engineering, University of Ljubljana in Ljubljana, Slovenia, where experimental investigations took place. The computer model of the unit was developed by the research team at the Brno University of Technology. As the starting point, the model previously developed and tested in [10] was used. The model was further modified according to parameters of the storage unit located in Slovenia. Similarly as in [10], the quasi-2D structure of the model was proposed and implemented as a Type for the TRNSYS simulation tool. The effective heat capacity method was used for phase change modelling with the control volume method for the discretization of the governing heat transfer equation. The simulation model of the entire system consisting of the storage unit, the solar air collector, and other components was created in TRNSYS.

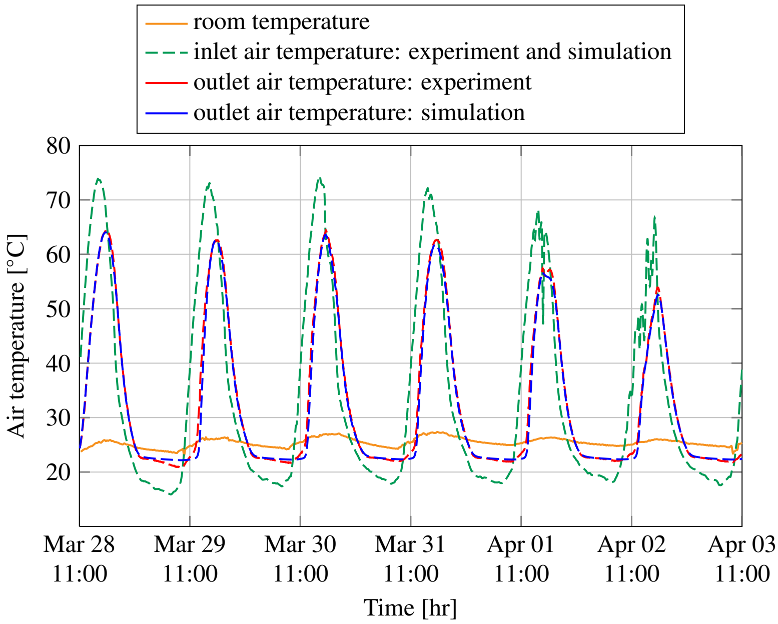


Figure 2.13: Comparison of the outlet air temperature: simulation vs. experiment [72]

The computer model was validated with the use of experimentally gained data by the team from Ljubljana. Figures 2.13 demonstrates good agreement between the model and experiment. Once the computer model was validated, the annual analysis of the performance of the heat storage unit was performed. The study was carried out for the heating season in Ljubljana from October to April. Weather data for a reference year available in the TRNSYS tool and provided by Meteonorm were used. The analysis identified that the highest coverage ratio of ventilation heat loss was 92% and 89% in April and in October, respectively, which are the months when the transition of seasons occurs. When considering the system with and without LHTES, the average coverage ratio for the heating season was 67% and 53%, respectively. Further, the economic analysis was performed to evaluate the annual cost savings. It was found that in case operating costs for energy use were the only costs taken into consideration, the system with LHTES allowed for 68% annual savings when compared to district heating.

Klimeš et al. [34]: Thermally activated wall panels with microencapsulated PCM: comparison of 2D and 3D models

The article [34] was concerned with computer modelling of a thermally activated building system (TABS) with a PCM. The considered TABS was a wall panel, which contained a plaster with a microencapsulated PCM. In the plaster, plastic tubes were embedded to allow the heat transfer fluid (water in the considered case) to flow through the tubes and thermally interact with the plaster, see Figure 2.14. The thickness of the plaster was 15 mm and the embedded tubes made of polyethylene had the inner diameter of 2.25 mm with the pitch of 15 mm between the tubes. Two modifications of the wall panels were investigated: the panel with straight tubes having the supply pipe at the top of the panel and the return pipe at the bottom of the panel, and the panel with U-shaped tubes having both the supply and return pipes at the top of the panel as shown in Figure 2.15.

Figure 2.14: Photograph of the experimental TABS. Left: the TABS before the application of the plaster, right: the complete TABS [34]

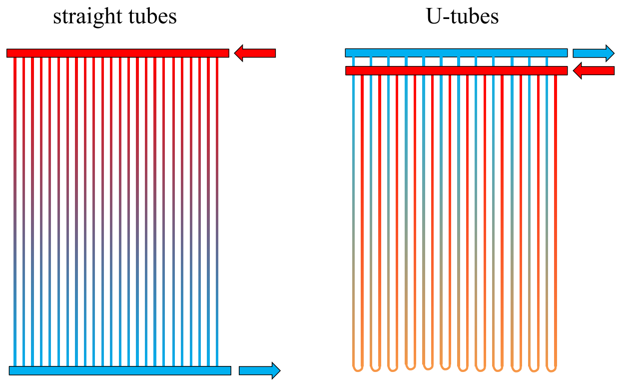


Figure 2.15: Two considered configurations of the TABS: straight and U-shaped tubes [34]

The main aim was to create a fast and accurate model of the TABS for the use in the TRNSYS simulation tool. The motivation was that though some off-the-self commercial packages are available for the coupled heat transfer and fluid flow problem involved in the considered TABS operation, due to huge computational costs those computational tools are suitable for simulations of only one wall panel rather that for overall simulations and analyses of rooms and buildings employing a number of the TABS. The model was developed and its functionality in terms of accuracy and computational efficiency was assessed by means of the comparison with the model created in COMSOL Multiphysics. The developed model for TRNSYS was based on the quasi-2D approach, while the model in COMSOL was fully 3D. The model for TRNSYS was implemented in C++ and it used the control volume method for the spatial discretization. The effective heat capacity method was employed for the phase change modelling. The non-isothermal fluid flow in the tubes was solved by means of balance-based interactions between the 1D heat transfer sub-models for the plaster with the PCM and the sub-model for the fluid flow in the embedded pipes. On the other hand, the model in COMSOL considered 3D heat transfer with the effective heat capacity and the non-isothermal laminar fluid flow, which were coupled together by means of the multiphysical interface.

It was found that the model for TRNSYS is much faster than the model created in COMSOL, which makes it applicable for TRNSYS simulations within large time scales. As for the computational accuracy, a very good agreement between the models was identified. In case of panels with the straight tubes, a very good accuracy was attained for all the considered flow rates of the heat transfer fluid. In case of panels with the U-shaped tubes, some discrepancies were observed for flow rates below 0.5 ml/s. Figure 2.16 shows simulation results for the mean surface temperature of the TABS with a very good agreement between the models.

Charvát et al. [11]: Utilization of an air-PCM heat exchanger in passive cooling of buildings: A simulation study on the energy saving potential in different European climates

In the paper [11], the energy saving potential for passive cooling of buildings by means of the air-PCM cold storage unit previously studied experimentally as well as numerically in [10, 72] was in-

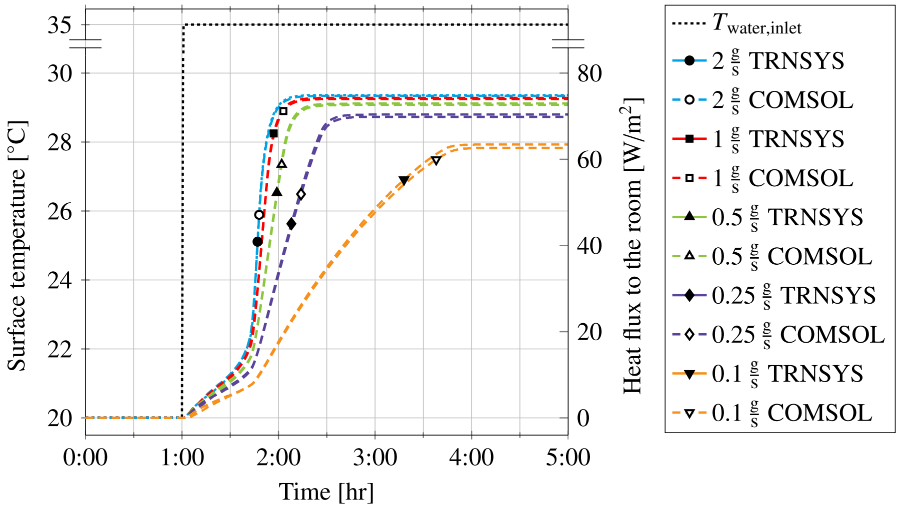


Figure 2.16: Surface temperature of the TABS with straight tubes: a very good agreement between the quasi-2D model for TRNSYS and the 3D model in COMSOL [34]

vestigated by means of computer simulations. During the daytime, the cold storage unit was utilised to cool down the outdoor air supplied to a building. On the other hand, heat stored in the PCM during the day was discharged (and thus cold was accumulated) to the outdoor environment during the night. The analysis was carried for sixteen cities in the Europe in the period between May 1 and September 30, and six mean phase change temperatures in the temperature range between 16 °C and 26 °C were taken into consideration. The temperature threshold of 20 °C was used as a switch for the utilisation and discharging of cold stored in the unit. One of aims of the study was to determine the optimal mean phase change temperature for each location, ranging from Athens as the southernmost considered city to Helsinki as the northernmost considered city.

The results showed that the dependence of the energy saving potential on the location of the city was not as significant as could be expected. In case of Athens, approximately a 30% higher energy saving potential was identified in comparison to Helsinki. Madrid was identified as the city where the maximum energy saving potential of about 190 kWh can be obtained in the investigated period for the mean phase change temperature of 24 °C. The average value of the utilisation rate of the heat of fusion, which was defined as the ratio between the energy saving potential in a 24-hour cold storage cycle and the heat of fusion of the PCM accommodated in the storage unit, did not exceed 50% in any configuration, but in about 10 days the value of the utilisation rate of the heat of fusion exceeded 90%. Further, the economic assessment of the use of the cold storage unit for passive cooling was performed. However, considering the price of 10 Euro per one CSM panel, the simple payback time of the cold storage unit would be well beyond the expected lifespan of the cold storage unit. Its economic viability is therefore crucially dependent on the price of the PCM: a significant reduction of its price would make PCM-based devices economically viable.

Pospíšil et al. [62]: Energy demand of liquefaction and regasification of natural gas and the potential of LNG for operative thermal energy storage

The paper [62] was aimed at the assessment of energy demands of liquefaction and regasification processes of the natural gas (NG) and at the evaluation of the potential of the liquefied natural gas (LNG) for operative thermal energy storage. The LNG process is fairly energy demanding and it consists of the liquefaction of the NG, transportation and storage of the LNG, and the regasification of the LNG into the NG. Methods available for these three processes were analysed. The study was particularly concerned with the assessment of the chain of energy transformations involved in the LNG process. Two views to the process were evaluated: the utilisation of the LNG for direct thermal energy storage of cold, and the utilisation of the LNG for indirect storage of power. The results showed that the overall efficiency of the use of LNG for energy storage is significantly dependent on particular technologies involved in the chain of LNG process as well as on the total capacity considered in a particular case. If energy-efficient liquefaction and regasification technologies are employed, then it is possible to use the LNG as an energy storage medium in an effective way.

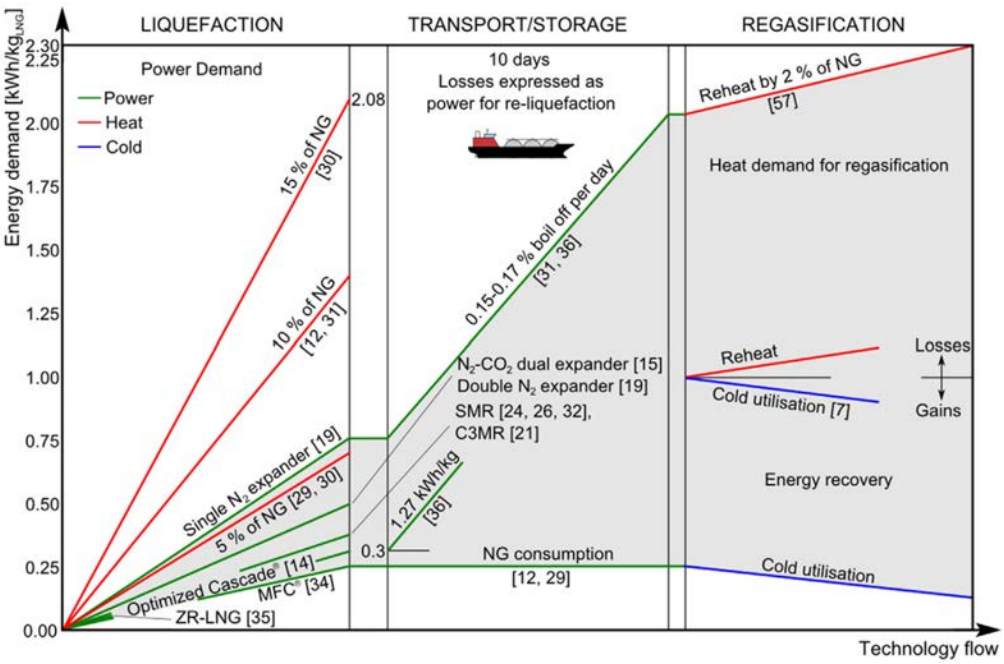


Figure 2.17: Analysis of energy demands in the LNG process [62]

Figure 2.17 shows the diagram with the graphical representation of energy demands (grey area in the diagram) and gains in the LNG process. The upper piece-wise line boundary of the grey area represents the most energy demanding LNG process with about 2.3 kWh/kg$_{LNG}$, which corresponds to about 20% consumption of LNG. On the other hand, the lower piece-wise line boundary of the grey area indicates the LNG technology, which is the most effective in terms of minimum consumption of energy, as well as of maximum regeneration of energy from the cold stored in the LNG. This most effective LNG technology is represented by the MFC (Mixed Fluid Cascade) liquefaction process with the energy demand of about 0.25 kWh/kg$_{LNG}$, the transportation of the LNG without the need for the LNG re-liquefaction, and the energy recovery from the cold and the power generation in expanders and turbines during the regasification process.

3 Phase change modelling and process control in steel production

Metal processing and steel production represent an important industrial application, in which the phase change and the latent heat significantly influence the solidification of metals, and mechanical and physical properties of finished products. At the moment, more than 98% of the total world production (TWP) of steel, aluminium, as well as copper is cast by means of the continuous casting method [86]. Though the TWP of steel is increasing every year, steelmakers at steel plants rather aim at the production of high-quality and high-alloyed steel grades having an extra added value for customers [77]. Examples of such grades include steel grades, which are used for the production of shells of boilers and pressure vessels, micro-alloyed steel grades, or highly resistant steel grades for the use in off-shore constructions in aggressive salt water on coast sides. Another view includes environmental impacts of the steel production to the natural environment and their minimisation.

3.1 Continuous steel casting

The continuous casting method [46] shown in Figure 3.1 is based on uninterrupted casting of the molten steel into the water-cooled mould, from which a semi-continuous steel strand with the solidified shell on its surface, but with a liquid core continues to the secondary cooling zone. In the secondary cooling zone, the solidification and cooling proceed due to water or air-mist spraying nozzles, which withdraw heat from the steel strand by means of the forced convection, and due to radiation to the ambient environment. The cooling process and its distribution in the mould and in the secondary cooling zone greatly influence the quality of steel products, including material as well as mechanical properties. A great attention is paid by steelmakers to surface and internal defects [52, 17], which may cause the rejection of the cast strand from next processing, meaning a higher scrap ratio, and thus a lower yield.

Recently, the production of high quality steel grades in a way reducing impacts to the natural environment cannot be accomplished without deep knowledge of the solidification process and its computer simulation and prediction. The literature review [77] on the current state-of-the-art in the steel production demonstrates that the casting process with no support in terms of computer simulations and of process control by means of computer models is inefficient, with a high occurrence of quality defects and other issues. Therefore, computer models are currently widely utilised at steel plants for monitoring of casting process, for the investigation of influences of process parameters, for the determination of optimal casting parameters, and for the real-time casting control and optimisation. The current research in the field of computer simulations of continuous steel casting mainly focuses on the development of models taking into account specific phenomena, such as the fluid flow prediction of the melt in the mould and in the liquid core of steel strand [58], fluid flow induced by the electromagnetic stirring [50], coupled thermal-mechanical phenomena encountered in the soft reduction method [30], or coupled thermal-mechanical-material phenomena in the prediction of cracks and other defects [61], which can arise during the production due to an improper setup of the casting machine and due to improper operational parameters of the casting process. Another issue is computer modelling of near-net-shape casting [46], in which a very high casting speed requires special numerical techniques providing the numerical stability of computer models.

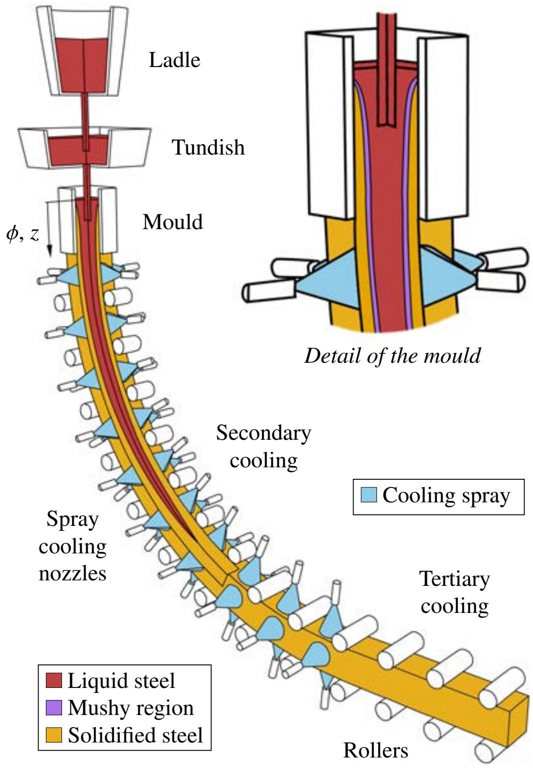


Figure 3.1: Schematic of continuous steel casting [38]

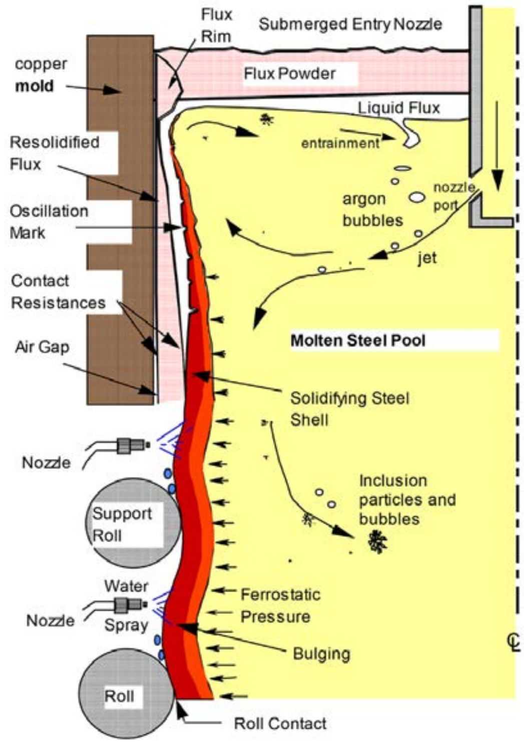


Figure 3.2: Multiphysical phenomena in continuous steel casting [76]

3.2 Computer modelling of continuous steel casting

A number of researchers and investigators have contributed to the field of computer modelling of continuous steel casting and to the use of computer models in the casting control and optimisation. This section briefly summarises some achievements and the current state-of-the-art. When considering the purpose of the models, they can be split into two main groups [77]: simpler and fast models for the use in real-time monitoring, control, and optimisation of the casting process, and more complicated and complex models, which enable detailed analyses and simulations of multiple phenomena. However, such detailed models are computationally expensive and often very slow, which makes them not applicable for the real-time use.

3.3 Heat transfer and solidification models and phase change modelling

Computer modelling of continuous steel casting consists of the numerical solution of a coupled multiphysical problem incorporating heat transfer, mass transfer with fluid flow, and phase changes [46] as demonstrated in Figure 3.2. The heat transfer phenomena are rather obvious: the primary task in continuous steel casting is a controlled transformation—the solidification—of the liquid steel into semi-finished products in the solid state. During the solidification, a vast amount of heat needs to be withdrawn from the strand to the ambient environment. As for the heat transfer mechanisms, all three kinds are taken into account: heat conduction as the dominant heat transfer mechanism in the solidifying strand, while heat convection and radiation are crucial mechanisms serving as boundary conditions (forced convection induced by spray nozzles in the secondary cooling zone, and natural convection and radiation in the tertiary cooling zone.

As for mass transfer and fluid flow, they are mostly involved in the mould and in the liquid core of the strand. Especially in the investigation of electromagnetic stirring and submerged entry nozzles, fluid flow needs to be solved. However, since the viscosity of the liquid steel is rather high, a number of authors of computers models for continuous steel casting have applied a simplified approach, in which the fluid flow is solved and accounted indirectly, often by means of the concept of effective thermal conductivity [47, 49], instead of the direct solution of the Navier-Stokes equations. A direct solution of the fluid flow takes place particularly in specific models of the mould, where the strand exiting the mould is not further considered and simulated. Another important aspect in the solidification of steel and its computer modelling is the phase change. The phase change, besides the influence to mechanical and physical properties and to the structure, is accompanied by the release of a large amount of heat in a relatively narrow temperature interval. In case of low-alloyed carbon steel grades, there are usually two phase changes during the solidification: the liquid-to-solid phase change (the solidification itself) and solid-to-solid transformations in the solid state accompanied by changes of the structure [78].

Though the currently utilised computer models particularly include the above mentioned phenomena, their list to the relation of continuous steel casting is not complete as illustrated in Figure 3.2. Nowadays, there are challenging efforts to develop even more complex models, which would encompass multidisciplinary effects ranging from multiphase turbulent flow and electromagnetic effects to particle entrapment to clogging and to segregation and micro-structure formation [77]. Coupled thermal-mechanical or thermal-structural models are of particular interest, though they are in general rather in a development stage.

Thermal models with phase change

In heat transfer modelling of continuous steel casting, there are two main categories of modelling approaches applied by investigator and developers of the models. The first category consists of mathematical and numerical methods, which are rather simpler and straightforwardly implementable. Methods from this category [73, 71] are frequently utilised in both academia and industry, and they represent the majority of the models. Another category includes advanced simulation methods, which are challenging from mathematical as well as programming/implementation point of view. Such methods [81, 41] are superficial in some aspects when compared to standard methods; however their complexity, requirements, and computational costs are well beyond the standard methods. Such models are utilised predominantly in academia for research purposes with a rather limited use in industrial applications at steel plants. When considering straightforward methods for implementation of the thermal model with the phase changes, the enthalpy method [73] and the effective heat capacity method [71] are two frequently utilised techniques. Both the methods are grid-based under the Euler principle, well suitable and thus frequently applied to computer modelling of continuous steel casting.

Enthalpy method. The method is based on the use of the thermodynamic enthalpy, which allows for the inclusion of both the sensible heat and the heat of fusion. The enthalpy H can be defined [73] as a function of the temperature T according to

$$H(T) = \int_{T_{\mathrm{ref}}}^{T} \left(\varrho c_p - \varrho \Delta H_{\mathrm{m}} \frac{\partial f_{\mathrm{s}}}{\partial \vartheta} \right) \, \mathrm{d}\vartheta \tag{3.1}$$

where ϱ is the density, c_p is the heat capacity at constant pressure, ΔH_m is the heat of fusion, f_s is the solid fraction and T_ref is a reference temperature. The substitution of Eq. (3.1) to the heat transfer equation [29] (as already explained in Section 2.5) and the consideration of the strand movement during the casting process lead to the governing enthalpy-formulated heat transfer equation [73]

$$\frac{\partial H}{\partial t} = \nabla \cdot (k \nabla T) + v_z \frac{\partial H}{\partial z} \tag{3.2}$$

in the Cartesian coordinate system (x, y, z) with the assumption of z being the casting direction. In Eq. (3.2), t is time, v_z is the casting speed, and k stands for the thermal conductivity.

Effective heat capacity method. The method uses the heat capacity c_p, often referred to as the specific heat, for the inclusion of the heat of fusion. The effective heat capacity accounts as a function of the temperature $c_\mathrm{eff}(T)$ for both the sensible heat and the heat of fusion. The effective heat capacity is related to the enthalpy as [71]

$$c_\mathrm{eff} = \frac{1}{\varrho} \frac{\partial H}{\partial T} = c_p - \Delta H_\mathrm{m} \frac{\partial f_\mathrm{s}}{\partial T}. \tag{3.3}$$

Similarly as in case of the enthalpy method, the substitution of Eq. (3.3) to the heat transfer equation [29] and taking into account the casting speed lead to the governing effective-heat-capacity-formulated heat transfer equation [68]

$$\varrho c_\mathrm{eff} \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + v_z \varrho c_\mathrm{eff} \frac{\partial T}{\partial z}. \tag{3.4}$$

The governing equations (3.2) and (3.4) formulated with the use of the enthalpy method and the effective heat capacity method, respectively, are the most frequently implemented techniques in computer models of continuous steel casting, both in research papers (e.g. [59, 68, 27]) as well as in industry (e.g. ProCAST software [53]). The reason is that both the methods are relatively simple, straightforwardly implementable and computationally efficient. Especially in case of the explicit formulation of the time discretization, their numerical solution does not require the solution of the set of equations, which might be an issue in case of a large number of computational nodes. As for the numerical formulation and the transition between the partial differential equations (3.2) and (3.4), and algebraic equations suitable for the numerical solution, the well-known and robust finite difference method, the finite volume method, and the control volume method (all already discussed in Section 2.5) can be applied.

As in case of modelling of LHTES systems, the enthalpy method offers a slightly better stability and accuracy than the effective heat capacity method, and it does not require methods for the energy conservation control since the enthalpy approach is self-conservative [55]. On the other hand, the enthalpy method requires a two-stage and computationally less effective solution for the two unknown variables H and T, while in case of the effective heat capacity method, T is the only unknown variable solved for.

Besides the enthalpy method and the effective heat capacity method, several other techniques are employed for computer modelling of continuous steel casting. However, their use is, in comparison to the enthalpy method and the effective heat capacity method, substantially less frequent in practical applications.

The thermal models are the most important simulation tool for the casting control and optimisation. The reason is that the temperature history and the location of the solidification front (iso-solidus and iso-liquidus cones) are directly connected to properties of final products as well as to the formation of defects. In contrast to most models aiming at specific phenomena as discussed in the foregoing section, thermal models are capable to operate in real time or even faster, which is crucial for the process optimisation and casting control. Therefore, a number of models with a different level of complexity and computational efficiency have been developed in the last two decades. Examples of the most well-known include the models CON1D [59], TEMPSIMU3D [47, 48], and models presented in [80] and [24].

Though the attention of investigators is at the moment focused mainly on modelling of specific phenomena, there is still an effort to the development devoted to the thermal models of continuous casting. For instance, a method for the reduction of complexity of the model for continuous steel casting was proposed by Mitchell and Vynnycky [54]. The authors claimed that the proposed technique allows for recovery of some fluid flow interactions only from the solution of the heat transfer model. Another example is the paper presented by Bratu at al. [7], in which the authors enhanced the heat transfer and solidification model by taking into account the convective heat transfer at the solid-liquid interface in the solidification region. Hietanen et al. [26] aimed at the solidification, heat transfer, and fluid flow modelling in continuous steel casting by means of an advanced modelling approach. The authors utilised ANSYS Fluent and an in-house heat transfer model TEMPSIMU3D, and they reported that the effective thermal conductivity taking into account fluid flow patterns of the liquid core can be applied in a sufficient accuracy only in region of the solidification end, whereas it is not applicable in locations where the liquid fraction is high.

3.4 Computer models in optimal control and optimisation of casting process

The main purpose of computer models of industrial processes is usually their use for process monitoring, control and optimisation, and for investigation of case studies. This also applies to continuous steel casting. Since the dynamic casting control makes sense especially in real time, rather simpler and sufficiently fast computer models are used for this purpose. On the other hand, the models can also be utilised in the off-line mode for the pre-calculation and determination of optimal casting parameters, and for case studies.

Use of mathematical programming techniques

Methods based on mathematical programming have been mainly utilised in scheduling problems. Jiang et al. [31] presented a solution of the scheduling problem for continuous steel casting, which consisted of cost and penalty objectives. The authors proposed a prediction-based online soft scheduling algorithm and they reported that the algorithm outperforms other algorithms and allows for an approximate determination of the cost objective. In further work, Jiang et al. [32] presented a multi-stage dynamic soft scheduling algorithm, which was based on an improved differential evolution. The uncertainty was taken into account by means of the scenario-based approach and the decomposition was used for the solution of the problem. Similarly as in [31], the authors reported that the proposed algorithm is more efficient than other algorithms.

Use of meta-heuristics and nature-based algorithms

The range of applications of meta-heuristics in optimisation of continuous steel casting is rather wide ranging from scheduling to the process control. Santos et al. [67] created a control system based on heuristic search techniques and a genetic algorithm. The aim was to maximise the production rate and the system was proposed to determine optimal parameters including water flow rates in the secondary cooling zone. The applicability of the system was demonstrated with the use of experimental data, and it was shown that modifications suggested by the model led to the reduction of the water consumption and to an assured strand quality. Hetmaniok et al. [25] proposed a method for the restoration of cooling conditions in the mould and in the secondary cooling zone. The authors employed the alternating phase truncation method for the solution of a direct heat transfer problem, and the ant colony algorithm and the artificial bee colony algorithm were used for the minimisation of errors between simulation and experimental results. A good agreement and efficiency of the method were reported.

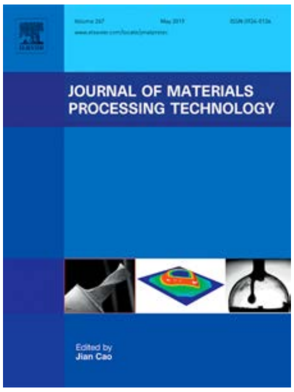
Use of other control algorithms

Petrus et al. [59] presented a control algorithm of spray cooling in the secondary cooling zone by means of a 1D finite difference heat transfer model of continuously cast steel strands. The authors reported that the algorithm is capable for the real-time operation. Furtmüller et al. [21] addressed the stabilisation of dynamic bulging (large oscillations of the level in the mould) by means of an adaptive robust stabilisation. The adaptive control method was proposed for the reduction of dynamic bulging without slowing down the casting process. The proposed method was validated with the use of experiments and its good applicability was reported. Liu and Xie [45] proposed a control system based on the fuzzy self-adaptive PID regulator, which aimed at the improvement of the billet quality and stability in the secondary cooling. The authors performed simulations as well as experimental investigations and it was reported that the fuzzy self-adaptive PID regulator outperformed other two considered controllers.

Rao et al. [63] utilised a teaching-learning-based approach for the parameter optimisation of casting parameters in continuous steel casting. The proposed model described a multi-objective multi-constrained problem and the authors reported that the proposed approach is more efficient when compared to the solution gained by means of the genetic algorithm. Wang et al. [83] presented a control algorithm for spray cooling in continuous steel casting, which was based on the use of the model-based predictive control method coupled with a particle swarm optimisation technique. The authors got their inspiration in the paper [38] since they created a GPU-based heat transfer model adopted from [38], and they used it in the model-based control algorithm as proposed in [37]. The authors reported that the proposed control system has a good computation performance and a satisfactory control performance.

3.5 Author's contribution to the development of modelling and control of continuous steel casting

Four journal papers co-authored by the author of the thesis and published in peer-review journals having the impact factor according to Web of Science are included in the thesis in order to demonstrate the author's contribution to the field of computer modelling, control, and casting analyses of continuous steel casting, which are based on the use of computer models. The journal papers included in the thesis are:

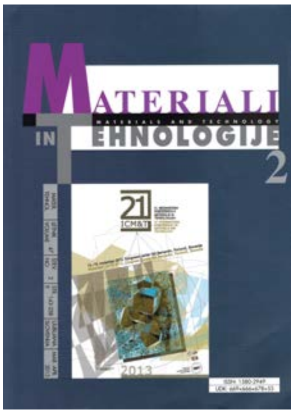


[38] Klimeš L, Štětina J. 2015. A rapid GPU-based heat transfer and solidification model for dynamic computer simulations of continuous steel casting. *Journal of Materials Processing Technology* **226**: 1–14.

Author's contribution: 80%

Metrics: $\mathrm{IF}_{2015} = 2.36$. $\mathrm{CiteScore}_{2015} = 2.90$. Citations: 19 (G Scholar).

Ranking: 2×Q1 and Q2 in JCR 2015 Web of Science.

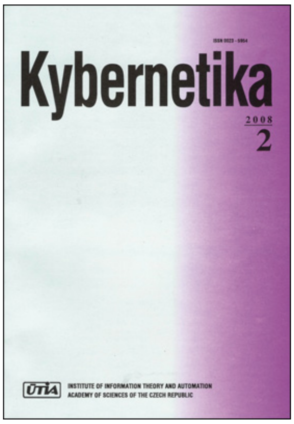


[39] Klimeš L, Štětina J, Buček P. 2013. Impact of casting speed on the temperature field of continuously cast steel billets. *Materials and Technology* **47** (4): 507–513.

Author's contribution: 75%

Metrics: $\mathrm{IF}_{2013} = 0.56$. $\mathrm{CiteScore}_{2013} = 0.69$. Citations: 6 (G Scholar).

Ranking: Q4 in JCR 2014 Web of Science.



[36] Klimeš L, Popela P, Mauder T, Štětina J, Charvát P. 2017. Two-stage stochastic programming approach to a PDE-constrained steel production problem with the moving interface. *Kybernetika* **53** (6): 1047–1070.

Author's contribution: 50%

Metrics: $\mathrm{IF}_{2017} = 0.63$. $\mathrm{CiteScore}_{2017} = 0.62$. Citations: 0.

Ranking: Q4 in JCR 2017 Web of Science.

[37] Klimeš L, Štětina J. 2014. Unsteady model-based predictive control of continuous steel casting by means of a very fast dynamic solidification model on a GPU. *Materials and Technology* **48** (4): 525–530.

Author's contribution: 80%

Metrics: $\mathrm{IF}_{2014} = 0.55$. $\mathrm{CiteScore}_{2014} = 0.89$. Citations: 3 (G Scholar).

Ranking: Q4 in JCR 2013 Web of Science.

Klimeš and Štětina [38]: A rapid GPU-based heat transfer and solidification model for dynamic computer simulations of continuous steel casting

The most significant achievement to the field of modelling and control of continuous steel casting was reported in [38]. The paper presented the development and benchmarking of the dynamic heat transfer and solidification model for continuous steel casting, which was designed for the use with graphics processing units (GPUs). A highly parallel code was proposed and implemented in CUDA/C++, which allowed for a very significant computational acceleration of the model in comparison to the state-of-the-art sequential CPU-based models for continuous steel casting. The developed GPU-based model utilised experimentally determined boundary conditions in the mould as well as for spray cooling in the secondary cooling zone. The functionality of the model was validated as well as verified according to experimental data from a steel plant and to an exact solution of the Stefan two-phase solidification problem, respectively. The computational performance of the GPU-based model was assessed and it was found that the use of GPUs allowed for the acceleration (when compared to a CPU-based model) between 33× and 68× for the grid having 100 thousand and 5 million computational nodes, respectively.

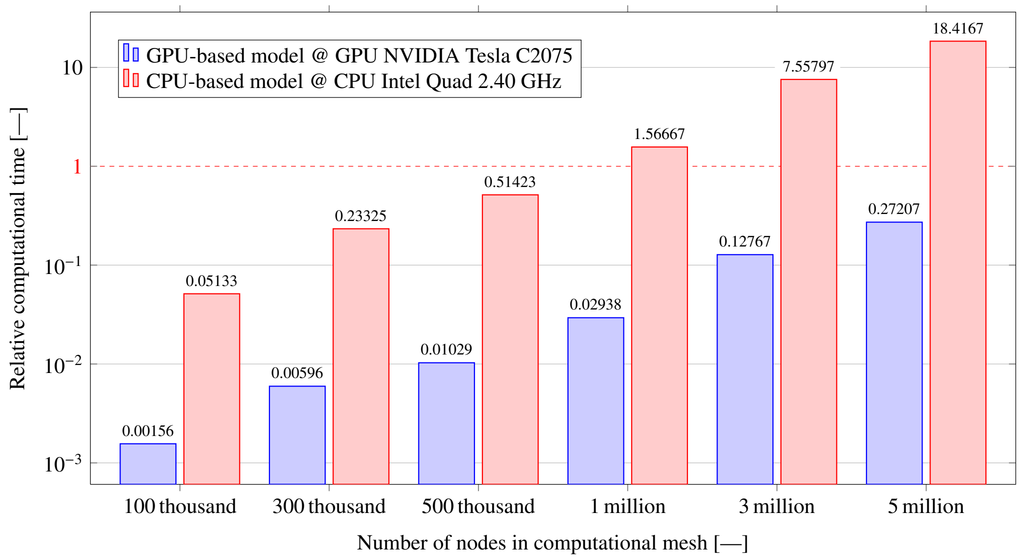


Figure 3.3: GPU-based model benchmarking—evaluation of the absolute computational time [38]

Figure 3.3 emphasises the advantage of the GPU-based model in case it is used in real-time control algorithms as a numerical sensor. In this case, the relative computational time is used to emphasise the necessity of fast models for their use in real-time optimisation and control systems. The reason is that in real-time control, the model needs to be faster or even much faster than the real wall-clock time as the control algorithm may require several evaluations of the model in order to determine the optimal control strategy for the next time instance. The paper [38] was already adopted by other authors [83], who re-implemented and adopted the model in their research work.

Klimeš et al. [39]: Impact of casting speed on the temperature field of continuously cast steel billets

The paper [39] was aimed at an analysis of thermal and solidification conditions in continuous casting of steel billets. The heat transfer and solidification model, which was based on the enthalpy

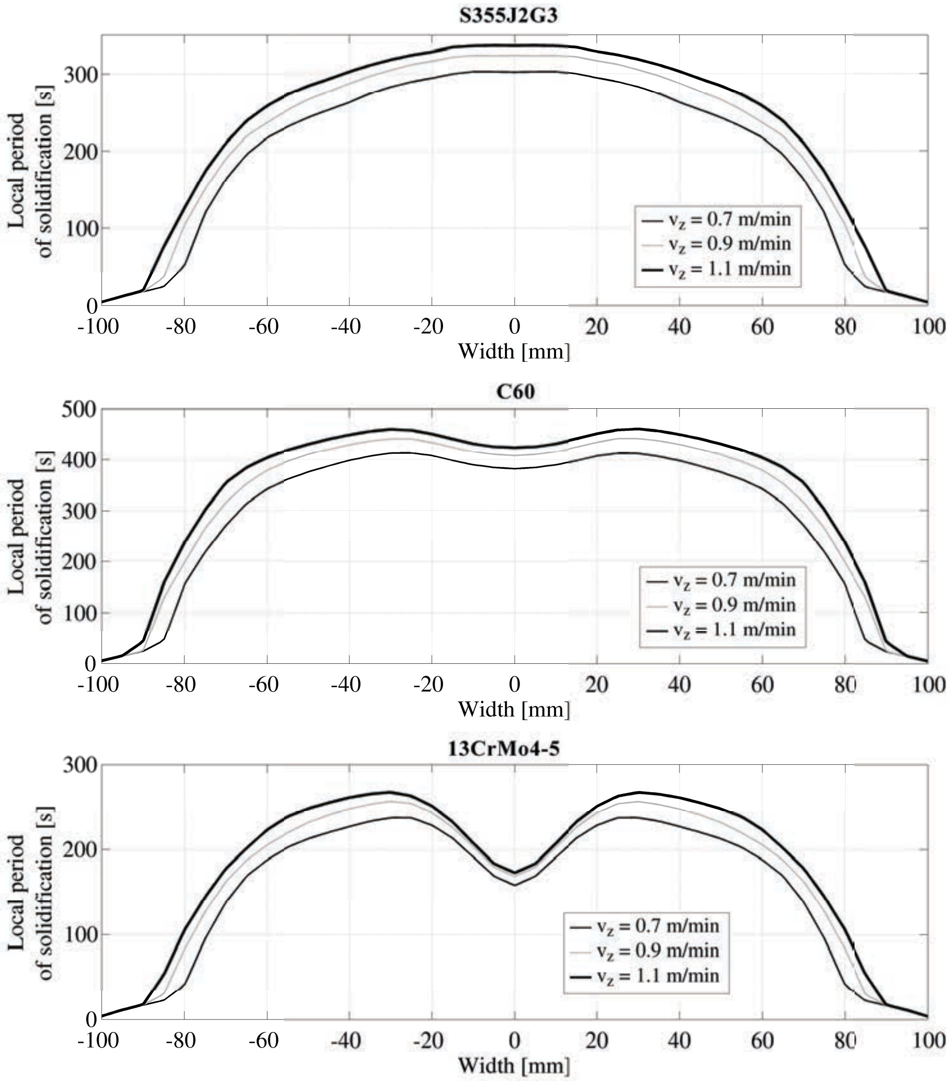


Figure 3.4: Computationally determined local time of solidification for various steel grades [39]

method and on the control volume discretization, was presented in the paper and its capabilities were demonstrated. Similarly as in [38], the model employs experimentally determined boundary conditions, and its functionality was validated by means of experiments and pyrometer measurements. In the paper [39], surface and corners temperatures, solidification regions, shell thickness, and the local period of solidification were computationally analysed for various casting speeds by means of the computer model. Such analysis enables metallurgists and cater operators for improvement of the strand quality, and for reduction of the occurrence of defects and quality issues. In particular, the temperature distribution at corners of the cast billets is directly related to the thermal stress and to the formation of cracks. Moreover, knowledge of the location of iso-solidus and iso-liquidus cones defining the distribution of the liquid and solid phases and their relationship to the location of the unbending point is crucial for the prediction of both internal and surface quality issues as reported in the literature. Figure 3.4 shows the local time of solidification, which expresses the duration of solidification across the strand cross-section. As can be seen from Figure 3.4, the local time of solidification for the carbon steel grade S355J2G3 has a typical parabolic character. However, in case of the alloyed steel grade 13CrMo4-5, the parabolic behaviour has a local drop in the centre of the billet, which can indicate a tendency to issues in the central part of the steel strand.

Klimeš et al. [36]: Two-stage stochastic programming approach to a PDE-constrained steel production problem with the moving interface

The paper [36] was concerned with techniques of mathematical programming for the optimal control of continuous steel casting under uncertainty. The stochastic programming approach, which uses random variables with a known probability distribution, was used for modelling of randomness. It is worth pointing out that almost all published papers were aimed at solution of deterministic problems, while the optimisation model in [36] allows for the consideration of random events.

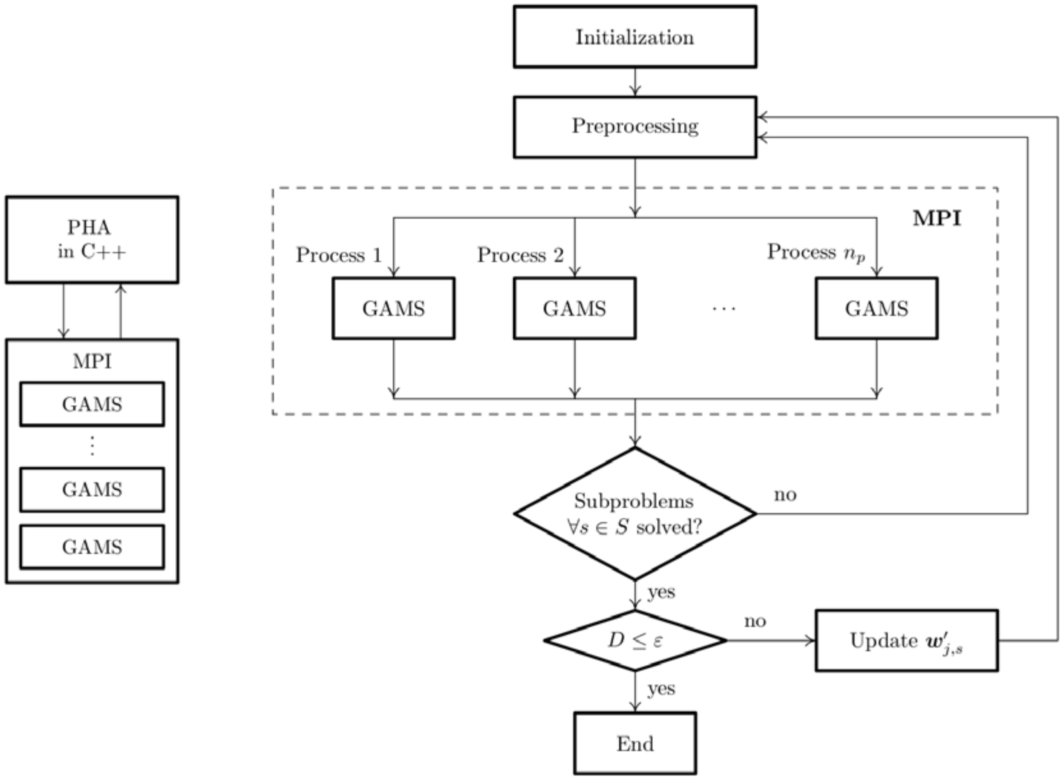


Figure 3.5: The block diagram and the flow chart of the parallel implementation of the progressive hedging algorithm [36]

The paper considered a two-stage decision making problem in the steel production. The randomness was used for modelling of a failure of the water pump in a loop in the secondary cooling zone, which would cause a sudden stop of spray cooling in the corresponding cooling loop. The scenario-based approach was utilised for modelling of randomness and the optimisation model was built in the general algebraic modelling system GAMS. The effective heat capacity method was used for the description of heat transfer and solidification of the steel strand, and the control volume method was applied to the formulation of discretized equations.

The scenario-based two-stage stochastic problem was solved with the use of the progressive hedging algorithm proposed in [64, 85], which was implemented as a standalone application written in C++. Since the solution of individual scenario-based problems was independent to each other, a decomposition and parallel solution was proposed and implemented by means of the message passing interface (MPI) API. The schematic of the implemented system is shown in Figure 3.5. The parallel decomposition was identified as an effective method for the reduction of the computational time needed for the solution of the problem. The stochastic optimisation problem with an uncertain fault of the pump was used for the demonstration of applicability of the proposed approach. The solution of the model resulted in a two-stage solution answering the following questions: "How to set up the casting speed and cooling conditions in the secondary cooling zone at the beginning of the casting process, which would maximise the casting rate, but taking into consideration a failure of the pump with a given probability? And in case the failure of the pump indeed happens, how to change the casting parameters to maintain the casting process in operation?" The optimisation case study was performed to answer these questions and the practicability of the determined solution was evaluated and assessed by means of quantitative characteristics.

Klimeš and Štětina [37]: Unsteady model-based predictive control of continuous steel casting by means of a very fast dynamic solidification model on a GPU

The paper [37] presented a dynamic control for continuous steel casting, which was based on the model-based predictive control (MPC) approach and on the use of the rapid GPU-based model presented in [38]. The very fast GPU-based model was a crucial part of the MPC mechanism: the control system used the GPU-based model for prediction of the future thermal behaviour of the strand in the so-called prediction (time) horizon.

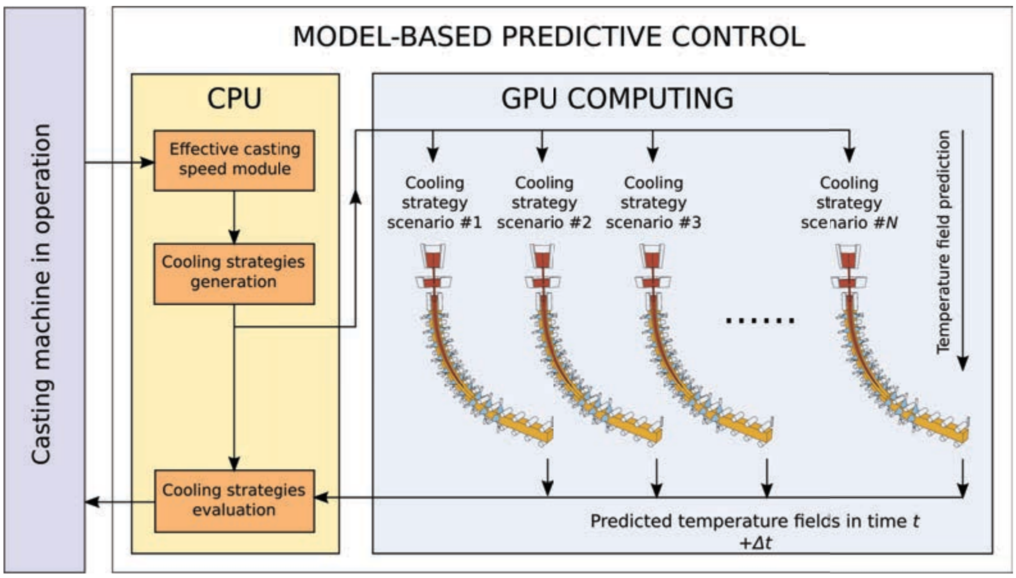


Figure 3.6: The schematic of the proposed MPC–GPU control system for continuous steel casting [37]

The underlying principle of the MPC was the fast evaluation of several cooling strategies (cooling scenarios), which were proposed and generated with the use of the effective casting speed. Since the GPU-based model is much faster that the wall-clock time, the GPU-based model allows for the pre-calculation and for the assessment of several cooling scenarios in real time. The schematic of the concept of the proposed MPC system is shown in Figure 3.6. It was shown that the proposed system has a good capability for the control of dynamic cases with strong changes of process parameters. The concept of the control system was further extended and validated in [33] where several case studies with dynamic changes of the casting speed were investigated, including the on-the-fly replacement of the tundish and the dynamic intervention of the breakout prediction system. The applicability and the proof of concept of the proposed control system were also confirmed by other investigators

[83], who were motivated by results presented in [37, 38] and who adopted the proposed control system bin their research work.

4 Conclusions and further work

Heat transfer with phase changes represents an important task in many technical applications and industrial processes. Nowadays, research and development not only in areas including heat transfer and phase changes are twofold: experimental and computational. In fact, these two approaches are commonly combined together as it is rather difficult to develop and optimise an engineering system just with the use of (usually expensive and time-consuming) experimental investigations, and similarly computer simulations without proper validation and verification by means of experimental data are hardly applicable as a reliable design and optimisation tool.

The thesis provides an insight into two areas, in which heat transfer with phase changes takes place: latent heat thermal energy storage (LHTES) employing phase change materials (PCMs), and the steelmaking process by means of continuous steel casting. The focus is concentrated on the computational solution and on the development of computer models of these systems, in which the phase change represents a crucial issue. Though the two applications may seem rather distinct at the first glance, they have many common properties, and similar modelling approaches can be applied to both of them. The contribution of the author to the field is demonstrated by ten journal papers, which are included in the thesis. Each paper co-authored by the author of the thesis has been published in a peer-review journal having an impact factor according to Web of Science.

LHTES represents a way for thermal energy storage by means of the latent heat accompanying the phase change. Suitable PCMs including e.g. paraffins and salt hydrates are often utilised in such systems. The latent heat (the heat of fusion) of the phase change is used to accumulate, store, and release heat. In the thesis, thermal storage units with a PCM designed for the use with solar air heaters, and a thermally activated building system containing a microencapsulated PCM were investigated by means of computer simulations. The effective heat capacity method and the enthalpy method were mostly used in the created models. However, it was found that the front tracking approach allows for about two orders of the magnitude higher computational accuracy, but its coding and implementation are significantly more challenging than in case of the commonly used enthalpy method and the effective heat capacity method. Further, the models were proposed and implemented in a way, which allows for their high computational efficiency. This means that they are well applicable for long-term simulations (the case of LHTES systems), and their computational efficiency makes them suitable for their coupling with optimisation algorithms. The developed computer models were validated with the use of experimental data or verified against other simulation data, and the models were used for analyses of the systems and their assessment and optimisation. In all cases, a good agreement between the created models and data from other sources was achieved. Further, it was concluded that LHTES and PCMs represent a viable way, which allows for efficient heat storage and for the utilisation of renewable energy resources (solar energy). In case of thermal storage units, their use enables the mitigation of mismatch between the energy demand and energy supply, for peak load shaving, and they can be used for ”free” cooling. In case of building structures, an integrated PCM allows for an improved thermal comfort, for preventing a room from overheating and temperature fluctuations, and for the increase of thermal inertial of lightweight buildings.

In case of steelmaking and continuous steel casting process, the phase change and the release of the heat of fusion during the solidification of steel represent an important issue, which needs to be properly addressed in computer modelling as well as in the real casting process. The reason is that the heat of fusion released during the solidification is a significant source of heat, which has to be withdrawn from the cast strand. Moreover, besides the liquid-to-solid phase change (the solidification), also solid-to-solid phase changes (e.g. the austenite–ferrite transformation) of steel has to be addressed properly in some cases. In recent years, the use of computer models for continuous steel casting is a common practice in research as well as directly in steel plants for the casting control and optimisation. In the thesis, the main achievement in modelling of continuous steel casting is the developed rapid GPU-based computer model, which enables very fast computer simulations allowing for the real-time casting control, e.g. by means of the model predictive control approach as demonstrated in the thesis. The GPU-based model provides the acceleration (when compared to a CPU-based model) in the order of tens (in particular, between $33\times$ and $68\times$ for the computational grid with 10^5 and $5 \cdot 10^6$ nodes). Further, it was also shown that stochastic programming is also applicable for optimisation of continuous steel casting under uncertainty, though not in the real-time use and having some limitations.

Various computer models and tools have been developed by the author for systems incorporating heat transfer with phase changes. As for the future work, the aim of the author is to continue with the improvement of existing models, and with the development of new models for other systems. Currently, two papers related to a computer model of the solar air collector with a PCM-based absorber and to a computer model of a PCM-based attenuator of the fluid temperature fluctuations are in a review process. Another objective of the further author's research will focus on optimisation: coupling of developed computer models with optimisation algorithms. The use of nature-inspired methods, metaheuristics and their implementations, e.g., in the open-source DEAP (Distributed Evolutionary Algorithms in Python) library for Python seem to be a promising way, already confirmed by results of other investigators.

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Computational heat transfer with phase changes in latent heat thermal energy storage and steelmaking

Abstract

Heat transfer and phase changes are encountered in many engineering applications and industrial processes. The thesis is aimed at the computational solution of heat transfer problems with phase changes in two technical areas: latent heat thermal energy storage with phase change materials and steelmaking by means of continuous steel casting. An insight into each area accompanied by the literature review of the current development in the field is provided, followed by several journal papers co-authored by the author of the thesis. Overall, ten journal papers published in peer-review journals having an impact factor in Web of Science are included in the thesis to demonstrate the author's contribution to the development in the fields. Achieved results indicate that the approach of computer modelling and developed models represent a viable way for effective design, optimisation, and control of the investigated systems.

Keywords: Heat transfer, phase change, computer modelling, latent heat thermal energy storage, phase change materials, continuous steel casting.

Výpočtové modelování přenosu tepla s fázovými přeměnami v úlohách akumulace tepla a výroby oceli

Abstrakt

Přenos tepla a fázové změny jsou významné děje zahrnuté v mnoha inženýrských aplikacích a průmyslových procesech. Tato práce je zaměřena na výpočtové modelování úloh přenosu tepla s fázovými přeměnami ve dvou technických aplikacích: akumulace tepla s využitím materiálů se změnou fáze a výroba oceli metodou plynulého odlévání. Pro každou oblast je v práci poskytnut přehled současného stavu vývoje a poznání, na který navazuje několik článků v časopisech, které demonstrují autorův přínos k vývoji v dané oblasti. Celkově je v práci zahrnuto deset článků, které byly publikovány v časopisech mající impakt faktor dle databáze Web of Science. Dosažené výsledky prokazují, že výpočtové modelování a vytvořené modely jsou vhodným nástrojem pro efektivní návrh, optimalizaci a řízení uvažovaných systémů.

Klíčová slova: Přenos tepla, změna fáze, výpočtové modelování, akumulace tepla, materiály se změnou fáze, plynulé odlévání oceli.