



BRNO UNIVERSITY OF TECHNOLOGY

VYSOKÉ UČENÍ TECHNICKÉ V BRNĚ

FACULTY OF MECHANICAL ENGINEERING

FAKULTA STROJNÍHO INŽENÝRSTVÍ

ENERGY INSTITUTE

ENERGETICKÝ ÚSTAV

**INVERSE IDENTIFICATION OF HYSTERESIS BEHAVIOUR
OF PARAFFIN-BASED PHASE CHANGE MATERIALS**

INVERZNÍ IDENTIFIKACE HYSTERZNÍHO CHOVÁNÍ MATERIÁLŮ SE ZMĚNOU SKUPENSTVÍ NA BÁZI
PARAFÍNU

DOCTORAL THESIS

DIZERTAČNÍ PRÁCE

AUTHOR

AUTOR PRÁCE

Ing. Martin Zálešák

SUPERVISOR

VEDOUCÍ PRÁCE

doc. Ing. Pavel Charvát, Ph.D.

BRNO 2024

KEYWORDS

Phase change hysteresis, phase change material, thermal energy storage, optimisation, inverse heat transfer problem

KLÍČOVÁ SLOVA

Hystereze změny skupenství, materiál s fázovou přeměnou, ukládání tepelné energie, optimalizace, inverzní úloha přenosu tepla

PLACE OF STORAGE OF THE DISSERTATION THESIS

Brno University of Technology, Faculty of Mechanical Engineering, Technická 2896/2, 616 69 Brno

MÍSTO ULOŽENÍ DIZERTAČNÍ PRÁCE

Fakulta strojního inženýrství VUT v Brně, Technická 2896/2, 616 69 Brno

Contents

Introduction	4
1. State of the art	5
1.1. Phase change hysteresis	5
1.1.1. Phase change hysteresis in complete phase change cycles	5
1.1.2. Phase change hysteresis in partial phase changes	8
1.1.3. Curve-track model	8
1.1.4. Curve-switch model	8
1.1.5. Isothermal and isoenthalpic toggling models	9
1.1.6. Curve-scale model	10
2. Analysis and conclusions of literature review	14
2.1. Approches to the numerical modelling of phase change hysteresis phenomena	14
2.1.1. One-curve model	14
2.1.2. Two-curve model	14
2.1.3. Partial phase change	15
2.1.4. Inverse problem	15
2.2. Scope of work in relation to the current state of knowledge	16
3. Aims of the study	17
3.1. Scientific questions and hypotheses	17
3.2. Thesis layout	18
4. Summary of conducted work	20
4.1. Paper [I.] (Research goals (A) and (C))	20
4.2. Paper [II.] (Research goals (B) and (C))	21
4.3. Paper [III.] (Research goals (A), (B), and (C))	23
4.4. Paper [IV.] (Research goal (C))	25
4.5. Paper [V.] (Research goal (C))	26
Conclusions	28
4.6. Future research	29
4.7. Limitations	29
References	30

INTRODUCTION

Phase change materials (PCMs) have gained a lot of attention in recent years, mainly due to their ability to store relatively high amounts of energy in a narrow temperature interval, making them a very promising technology for thermal energy storage applications [1]. At the same time, there is an ever-increasing need for means of renewable energy sources utilisation [2], which are inherently dependent on weather conditions, widening the gap between energy demand and supply. Such a problem encourages the development of systems with thermal energy storage (TES), which mitigates the energy supply/demand mismatch and improves the overall efficiency of the developed system. Applications utilising PCMs are taking advantage of the latent heat of phase change, which is either stored or recovered from the PCM during the phase transition process.

Considering an ideal scenario, the phase transition should take place at an exact specific temperature, but this is rarely the case [3]. PCMs usually undergo the phase transitions at a temperature interval rather than a defined temperature. In addition, it is necessary to consider phenomena such as phase change hysteresis (PCH) and supercooling (SC), which further complicate the thermal behaviour [4]. Several authors [5–7] have highlighted the importance of PCH in the numerical modelling of PCM thermal behaviour. The PCH phenomenon is usually undesirable since it limits PCM usage and may even be problematic if the PCH temperature shift is comparable to the order of working temperatures of a given device [4, 8]. The thermal behaviour gets further complicated in the case of the partial phase transitions, which occur when the phase transition is interrupted in the course of the heating/cooling process. The way in which this transition is conducted is crucial, and it has a profound effect on the overall thermal behaviour of a PCM, yet still, many authors are not considering this phenomenon in their calculations or using simplified modelling approaches [5, 9, 10]. This results in inaccurate temperature prediction, mainly in cases where cyclic changes of temperature near the phase change temperature are observed.

The main objective of this thesis was to investigate the thermal behaviour of PCM during the PCH numerically and experimentally. The state-of-the-art modelling approaches to the PCH during both complete and partial phase transitions were analysed, implemented in the form of a mathematical model and compared to each other. Experimental methods for the determination of effective heat capacity-temperature or enthalpy-temperature curves, such as differential scanning calorimetry or temperature-history methods, were used for validation of the developed PCH modelling methods. Furthermore, a framework for the identification of this behaviour, based on solutions to the inverse heat transfer problems (IHTPs), was developed utilising a wide range of solution methods.

1. STATE OF THE ART

The state-of-the-art literature review section concentrates on two primary areas of the thesis: the phenomenon of phase change hysteresis and the inverse problems associated with phase change modelling. These topics are inherently interconnected, as the former pertains to the thermal transfer mechanisms in PCMs, while the latter provides an explanation and solution for such behaviour. Further information about those topics can be found in recent review papers by Zálešák et al. [11] for inverse problem modelling and Klimeš et al. [9] for phase change hysteresis phenomena.

1.1. Phase change hysteresis

The thermal behaviour of PCMs has been the subject of extensive research over the past two decades. Compared to heat transfer without phase changes, there are two phenomena which further complicate the matter, introducing complexity to the behaviour of PCMs. These phenomena include phase change hysteresis (PCH) and supercooling (SC). To put it simply, phase change hysteresis disrupts the alignment of melting and solidification with their respective $h(T)$ or $c(T)$ curves [9] as shown in Figure 1.1.

The study by Jin et al. [12] investigated the melting/solidification processes for several PCMs. The results showed asymmetry in the processes for different PCMs, with some exhibiting high phase change hysteresis and supercooling (as shown in Figure 1.2). The findings suggest that the enthalpy of PCMs is influenced by their previous temperature states and applied heating/cooling rates.

1.1.1. Phase change hysteresis in complete phase change cycles

Goia et al. [5] have developed a numerical model of a PCM wall, which includes the PCH and compared the results obtained from simulation with experimental data. The proposed numerical model allows one to use separate enthalpy-temperature curves for heating and cooling, therefore improving the overall accuracy of the modelling approach. Both the heating and cooling curves were obtained by using the DSC method. The numerical model tracks the heating or cooling curve until the phase transition is completed (which is usually detected by reaching a specific temperature) and then transfers directly between the curves. A similar approach was adopted by many other authors [6, 10, 13], and the numerical model is often referred to as the two-curve model. EnergyPlusTM software was used for the model implementation.

Biswas et al. [10] adopted a similar approach. The authors developed a 2D numerical model of a wall with a PCM layer. PCMs based on fatty acids were chosen for investigation. Experimental measurements were carried out using the heat flow metre apparatus (HFMA) method. Toggling between the heating/cooling curves was allowed only in cases

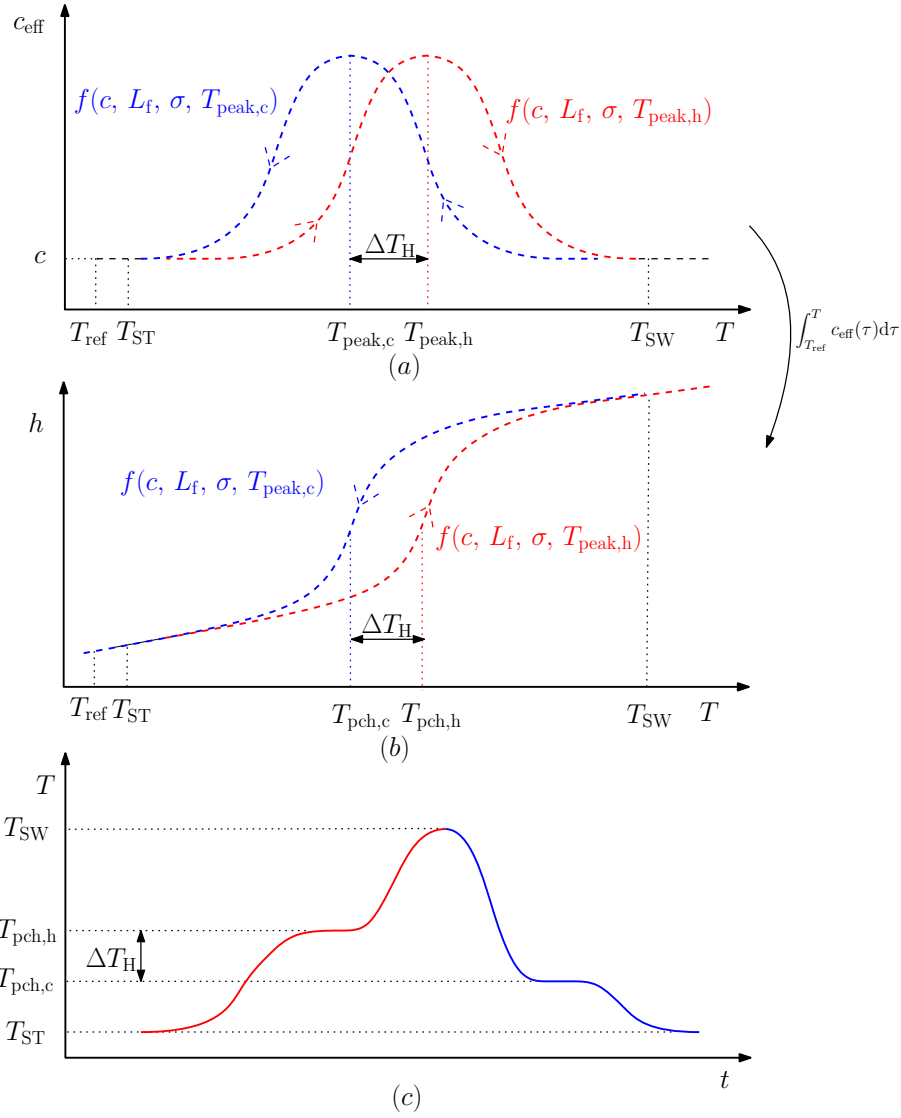


Figure 1.1: (a) Parameterization of the two-curve model with c_{eff} in the form of a Gaussian function, (b) enthalpy-temperature dependency $h(T)$, (c) Corresponding temperature-time relationship

when the temperature of the PCM left the phase change temperature region; therefore, toggling during partial phase changes was not allowed. A significant difference in thermal behaviour and energy savings was observed when the PCH was introduced into numerical modelling. In the case of the approach to modelling without PCH (using only the melting curve $h(T)$), energy savings of 32 % were observed (reducing the power consumption of the air conditioning). The authors have shown that when both heating and cooling curves were considered, the energy savings decreased to 29 %. Increasing the hysteresis shift by 2 °C and 4 °C led to further reduction of energy savings by up to 15 % and 12 %, respectively.

Stathopoulos et al. [13] developed a numerical model of an air-PCM heat exchanger (HEX) and a new calibration procedure using the effective heat capacity method. They found significant inaccuracies when using raw DSC data directly with a single $c(T)$ curve implementation. The calibration procedure aimed to optimize the shape of the function $c(T)$ while ensuring energy conservation, leading to the best agreement by considering three sets of heating/cooling curves and only reporting complete phase transitions.

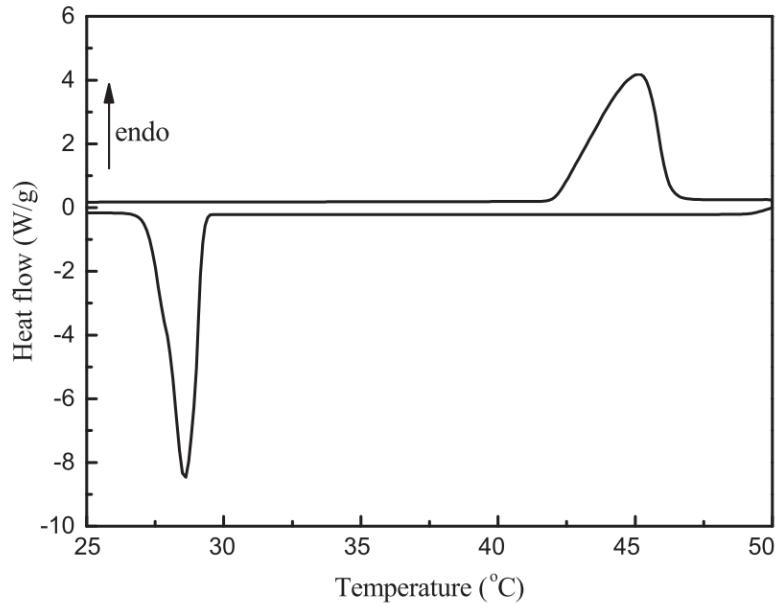


Figure 1.2: Heat flow - temperature dependency measured by dynamic DSC with 5 °C/min heating/cooling rate [12]

Moreles et al. [6] studied the influence of PCH on the thermal behaviour of a wall containing a layer of an organic macro-encapsulated BioPCM. The authors developed a 1D numerical model of heat transfer and coupled it with the effective heat capacity method, which was used for phase change modelling. The PCH was introduced, adopting the curve-track modelling approach. The melting curve was constructed based on data provided by the manufacturer, and the solidification curve was artificially defined by shifting the melting curve toward lower temperatures. The hysteresis temperature shift is equal to

$$\Delta T_H = T_m - T_s, \quad (1.1)$$

where T_m and T_s are the melting and solidification temperatures, respectively. The authors have investigated various degree of the PCH, ranging from the scenario without hysteresis ($\Delta T_H = 0^\circ\text{C}$) up to ($\Delta T_H = 30^\circ\text{C}$) and also different thicknesses of a PCM layer $e = 9 - 18$ mm. Unfortunately, similarly to the study by Stathopoulos et al. [13], only complete phase changes were considered. More research would be needed for partial phase changes. The results show improved thermal performance of a PCM wall with increasing hysteresis temperature shift, contrary to [10]. The authors also found that the best thermal performance occurred when the PCM underwent a phase transition outside the room's comfort temperature interval (17 – 23 °C).

Kuznik and Virgone [14] studied the thermal performance of a PCM wall, with the main objective of improving thermal comfort during summer and reducing energy consumption during winter. The effective heat capacity of a paraffin-based microencapsulated PCM (manufactured by ENERGAIN[®]) was investigated using the DSC method. The authors adopted the implicit finite difference method coupled with the effective heat capacity method for phase change modelling. Several different scenarios (one-time melting, one-time solidification, and consecutive melting followed by solidification) were investigated using only the melting or solidification effective heat capacity curve. Such an approach allowed to investigate the accuracy of simple one-curve models applied to more complex cyclic scenarios, where PCH is introduced. The results have shown that the sin-

gle effective heat capacity (melting or solidification) is not sufficient to describe thermal behaviour when compared with the experimental temperature data for one-time melting and solidification. Furthermore, neither of the effective heat capacity curves provided an accurate temperature prediction in case of consecutive melting and solidification. These results emphasise the importance of PCH and recommend it as a mandatory part of phase change modelling.

Table 1.1: Overview of research works related to complete phase changes

Reference	Year	PCH modelling approach	Validation of PCH	Parametrisation
Biswas et al. [10]	2018	Heating & cooling curve	✓	HFMA measurement
Goia et al. [5]	2018	Heating & cooling curve	✓	Data from manufacturer (measured with 3-layer-calorimeter)
Jin et al. [12]	2015	Experimental study	✗	DSC measurement
Kuznik and Virgone [14]	2009	Heating & cooling curve	✓	DSC measurement
Moreles et al. [6]	2018	Heating & cooling curve	✗	Linear interpolation
Stathopoulos et al. [13]	2017	Multiple $c(T)$ curves	✓	Triangular step function

1.1.2. Phase change hysteresis in partial phase changes

A fundamental issue of the modelling of partial phase changes is the behaviour right after the transition between heating/cooling (melting/solidification) processes (considering that the process was interrupted inside of the 'mushy'-zone, which is a region where PCM is regarded as partially solid and partially liquid). It remains unclear whether the transition between heating and cooling curves should be made and, if so, in which direction and following what kind of curve. Various researchers have grappled with this transitional issue, and the following section explores the latest and most promising solutions to address this complex issue.

1.1.3. Curve-track model

The curve-track model, proposed by Chandrasekharan et al. [15], provides a simple method to address partial phase changes. It employs a single enthalpy curve throughout the entire phase transition, regardless of variations in heating or cooling within the 'mushy' region. The main limitation of the model lies in its suboptimal performance in describing phase change hysteresis during partial phase transitions [4–6]. However, scenarios involving partial phase change cycles hold significant relevance, particularly in the context of partial load operation in thermal storages employing PCMs [16].

1.1.4. Curve-switch model

Two modifications to the curve-track model have been suggested to model PCH during incomplete phase transitions [9]. The initial proposal, credited to Bony and Citherlet [17], involves incorporating a transition between the heating and cooling phase curves. Bony

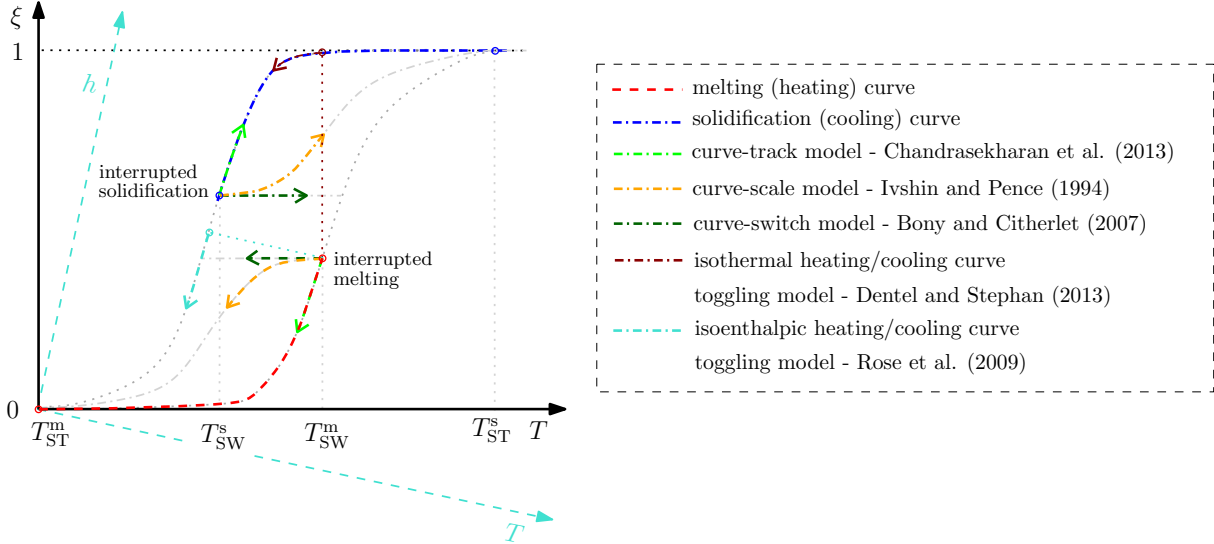


Figure 1.3: Approaches to the partial phase change modelling

and Citherlet [17] have conducted a study dealing with the development of a numerical model of heat transfer in a PCM placed inside a water storage tank. The TRNSYS software was used for the model implementation and an improved version of the curve-switch model was presented. The transition between heating and cooling curves was proposed following a straight line with the slope equal to the specific heat capacity in a solid/liquid state. These modified models are often referred to as curve-switch models [16]. The second modification is geared towards creating novel partial phase transition curves. These curves are situated within the hysteresis envelope, delineated by the curves representing complete phase transitions (the heating and cooling curves) [9]. This approach is often referred to as the curve-scale model and is described in further detail in the next section.

1.1.5. Isothermal and isenthalpic toggling models

Dentel and Stephan [18] introduced a 1D numerical model for wall constructions incorporating PCMs. This model, integrated as a user Type 399 in TRNSYS, is applicable for simulating both passive structures and thermally activated structures. The authors employed a direct toggling approach between the heating and cooling effective heat capacity curves as illustrated in Figure 1.3. Although Dentel and Stephan [18] did not validate the model, Delcroix et al. [19] conducted a further investigation in their study. They determined that the transition between the heating and cooling curves in this model was isothermal, resembling an instantaneous switch. This modelling approach is particularly suitable for scenarios involving complete phase change, where there is a minimal alteration in the effective heat capacity or enthalpy outside the phase change region. However, as demonstrated by Delcroix et al. [19], the toggling model is unsuitable for modelling of partial phase changes, as it violates energy conservation laws, leading to an overestimation or underestimation of the latent heat absorbed or released during the phase transition.

Rose et al. [20] created a computational model for building structures that integrates PCMs within BSim. The authors utilised a PCH modelling approach, relying on isenthalpic transitions between the heating and cooling curves. The model underwent validation through various case studies, demonstrating good applicability. Nonetheless,

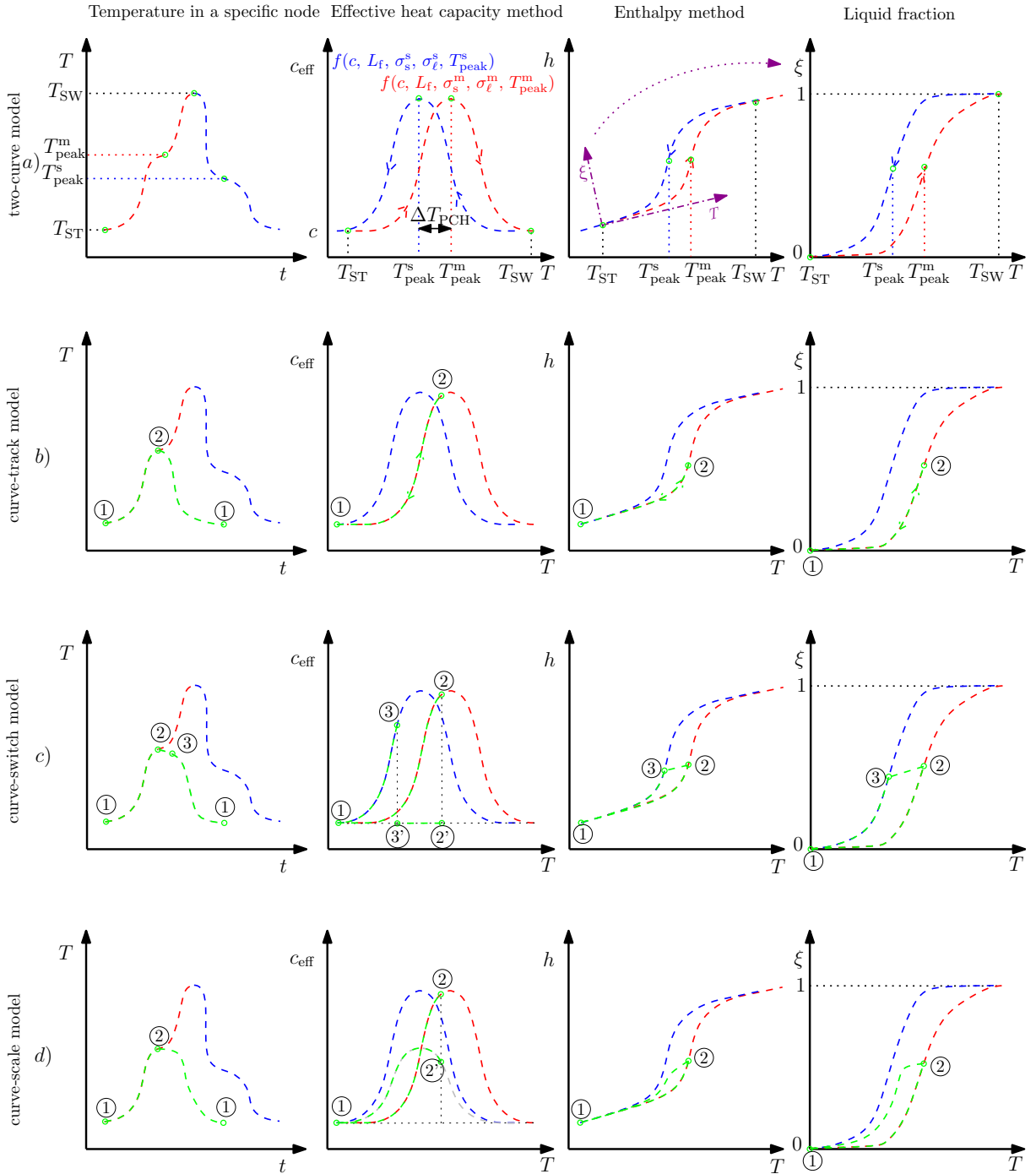


Figure 1.4: Modelling approaches to the partial melting of PCM – a) two-curve model b) curve-track model c) curve-switch model, and d) curve-scale model

its applicability tends to be rather specific, given that the examined dataset lacks any instances of partial phase change cycles.

1.1.6. Curve-scale model

The modelling methodology commonly known as the curve-scale model was initially conceptualized by Ivshin and Pence [21] in 1994. This model involves tracking the profile of the complementary curve (cooling curve for the partial melting cycle and heating curve for

the partial solidification cycle), originating from the point where melting/solidification was interrupted. The curve is then scaled down by a specific factor to ensure the smooth continuity of the liquid fraction of PCM. The authors have employed the Duhem-Madelung model, originally formulated for materials where multiple phases can coexist, forming a homogeneous mixture across a range of specific intensive thermodynamic quantities, such as temperature, stress, or magnetic field. Since its inception, numerous researchers have adopted this modelling approach with great accuracy [4, 16, 22].

Delcroix [23] proposed a hysteresis model addressing partial phase transformations in PCMs. A PCM was embedded in the wall structure, and phase transformation was induced. As the transformation progressed, the wall was subsequently moved to another room, and the material was left to solidify with natural convection. During this experiment, temperature histories were measured using several thermocouples, and data were subsequently utilised to validate the developed models. As was previously mentioned, the behaviour of PCMs when both phases coexist remains uncertain. An example is the case where PCM undergoes cooling only after partial melting, as illustrated in Figure 1.3. Upon heating PCM from state T_{ST} to state T_{SW} , several approaches can be considered to complete the hysteresis loop, i.e., the transition from state T_{SW} back to state T_{ST} . Bony and Citherlet [17] proposed transitioning to the cooling curve along a line with a slope corresponding to the specific heat capacity value in the solid/liquid phase (also referred to as wT , i.e., with transition). Another option (in this study referred to as noT - no transition, but otherwise called the curve-track model) was formulated by Chandrasekharan [15], suggesting staying on the heating curve during cooling. Delcroix [23] integrated these two approaches and validated them through the utilisation of experimental data.

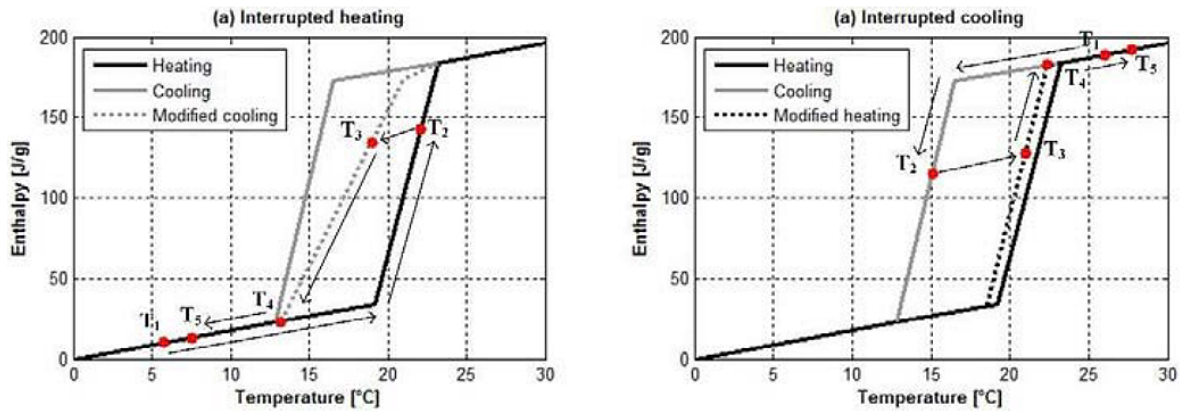


Figure 1.5: Transition between enthalpy curves for interrupted heating and cooling [23]

Furthermore, Delcroix [23] employed an optimization algorithm to determine the optimal shape of the enthalpy-temperature relationship for interrupted cooling and heating processes. The optimality criterion was based on the difference between experimental and simulation results. The optimal behaviour of PCM during hysteresis, as described by Delcroix et al. [23], is illustrated in Figure 1.5. Transitions between hysteresis curves occur along lines with slopes equal to the specific heat capacity [17]. In the case of interrupted heating, a transition to the cooling hysteresis curve occurs, positioned between the melting and solidification curves. Conversely, during interrupted cooling, heating follows the melting curve, as depicted in Figure 1.5.

In 2017, Delcroix et al. expanded their work from 2015 [19]. They developed a wall model with PCM incorporating hysteresis, time-varying physical constants, and super-

cooling. This model was integrated into TRNSYS software as Type 3258. Figure 1.6 illustrates the relationship between enthalpy and temperature, depicting the behaviour of PCM during phase change. Curves 1 and 2 represent the heating and cooling processes, while Region 3 can only be reached during interrupted heating or cooling Delcroix et al. [23]. Curve 4 describes PCM behaviour during supercooling, a phenomenon where the material is cooled below the solidification temperature and then rapidly crystallizes, resulting in a steep temperature rise. This state can occur only if the PCM is fully in the liquid phase and undergoes gradual cooling. The last region, Region 5, corresponds to interrupted supercooling, where new temperatures are calculated based on the specific heat capacity in the liquid phase.

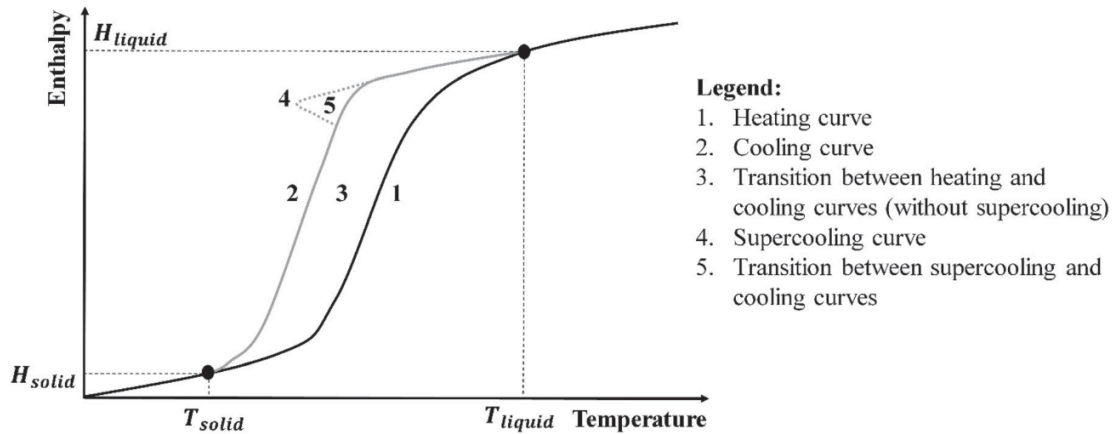


Figure 1.6: Description of regions in the enthalpy-temperature relationship utilized in the simulation [19]

Barz and Sommer [4] undertook a comprehensive investigation focused on modelling approaches for PCH. The study presented a phenomenological perspective on the PCH phenomenon, wherein the toggling strategy between heating and cooling curves was not only defined but also implicitly described through mathematical equations. Four distinct modelling approaches were explored: a static direct mapping model (SDMM), a static hysteresis model (SHM), a melting/solidification kinetic model (MSKM), and a solidification kinetic model (SKM). The four proposed models underwent comparison with experimental data, utilizing a tube-in-tube heat exchanger as the subject device. Results revealed notable discrepancies for the SDMM, attributed to its omission of PCH considerations. The SHM demonstrated significantly improved results. The rate-dependent PCH models (MSKM, SKM) exhibited even better agreement with experimental data, albeit necessitating additional experimental data for parametrization. The authors concluded that, for practical applications, the SHM presented the optimal compromise among the four modelling approaches considered.

Thonon et al. [22] conducted a comprehensive examination of the thermal characteristics of PCMs, specifically addressing phase change hysteresis and supercooling in both complete and partial phase change cycles. The study involved subjecting a test rig with a polymer-based PEG6000 PCM to heating and cooling cycles. Measurements of the PCM temperature and heat flux on the outer surfaces of a PCM sample were recorded, facilitating a thorough thermal characterization. The collected experimental data were used in an optimization procedure employing two objective functions: the RMSE between simulated and measured temperatures/heat fluxes. The optimization was carried out using

a genetic algorithm (GA). A Pareto front was employed to handle uncertainties stemming from experimental measurements. The authors reported good agreement in cases involving complete phase change and partial solidification cycles. The curve-scale partial phase change modelling technique was identified as the optimal approach for describing the thermal behaviour of the studied PCM.

Table 1.2: Overview of research works related to partial phase changes

Reference	Year	PCH modelling approach	Basic principle of phase change modelling
Barz and Sommer [4]	2018	Two rate-dependent and two rate-independent phenomenological approaches	The models are formulated by integrating distinct elements from various approaches
Bony and Citherlet [17]	2007	Curve-switch	The transition between the melting and solidification curves exhibits a linear decline with a slope equivalent to the specific heat capacity c
Chandrasekharan et al. [15]	2013	Curve-track	No transition occurs between the melting and solidification curves until the phase transition of the PCM is complete
Delcroix et al. [23]	2015	Curve-switch, curve-track, and adaptation of curve-scale	A simplified piece-wise linear version of the curve-scale approach is used in the study. Transitional behaviour is defined according to Bony and Citherlet [17] in case of the Curve-switch approach and Chandrasekharan et al. [15] in case of the curve-track approach
Delcroix et al. [19]	2017	Curve-switch and curve-track	Both approaches are based on the original research by Bony and Citherlet [17] and Chandrasekharan et al. [15]
Dentel and Stephan [18]	2013	Isothermal toggling	Instantaneous switching between the melting and solidification curves in the isothermal direction
Rose et al. [20]	2009	Isoenthalpic toggling	Instantaneous switching between the melting and solidification curves in the isoenthalpic direction
Thonon et al. [22]	2021	Curve-scale	Following partial solidification and partial melting, a reduced-scale representation of the melting/solidification curve is employed

2. ANALYSIS AND CONCLUSIONS OF LITERATURE REVIEW

2.1. Approches to the numerical modelling of phase change hysteresis phenomena

The authors primarily employ methods based on effective heat capacity and enthalpy. The effective heat capacity method (c_{eff}) is generally easier to implement and computationally faster; however, with increasing time discretization steps, it may yield inaccurate results and encounter issues with numerical stability [24]. Conversely, the enthalpy method is slightly more computationally demanding but numerically more stable. Hysteresis can be described using both of these methods, making it a matter of preference depending on the specific problem. The numerical model is largely constructed by the authors as one-dimensional, aiming for reduced computational time and the symmetry inherent in the given problems. Most authors validate their models using experimental data for the specific device, although the literature review also includes purely theoretical articles.

2.1.1. One-curve model

In the initial segment of the literature review, fundamental information was presented regarding materials undergoing phase transitions and the methodologies employed to model their behaviour. Presently, the basic forms of methods involving effective thermal capacity, enthalpy, or heat recovery have become standard tools in practice, with hysteresis being completely disregarded [5]. These models are referred to as one-curve models, as they utilize only a single curve representing the enthalpy-temperature relationship. However, this approach can lead to significant inaccuracies. For instance, inorganic phase change materials, especially those derived from hydrate salts, are known to exhibit notable hysteresis effects, with the temperature difference between the onset of melting and solidification phases extending to several degrees Celsius [25]. This oversight becomes particularly critical when accurate predictions of thermal performance are essential, emphasizing the need for more sophisticated modelling approaches that explicitly account for the PCH phenomenon.

2.1.2. Two-curve model

The majority of authors [5, 6, 10, 12–14, 26] describe hysteresis using two enthalpy-temperature curves. One curve corresponds to the heating/melting phase, while the other pertains to the cooling/solidification of the PCM. This model type is referred to as the two-curve model and provides a fundamental and intuitive representation of how

hysteresis occurs. This model has been verified against experimental data [5, 14, 19, 23, 26]. However, it exhibits agreement with experiments only for complete melting and solidification cycles [23]. In the case of incomplete cycles, a simple two-curve model fails to achieve agreement with measurements, revealing its incapacity to describe the behaviour of PCM during interrupted phase transitions [14].

2.1.3. Partial phase change

The modelling of partial phase transformations is well described by Delcroix [19, 23], building upon earlier works by other authors [15, 17]. The authors present two methods for transitioning between hysteresis curves (the heating and cooling curves): either along a line with the slope of the material's specific heat capacity [17] (often referred to as the curve-switch model), or back along the heating/cooling curve depending on whether it is interrupted heating/cooling [15] (also called the curve-track model). Delcroix et al. [23] successfully combined these approaches—transitions occur in the direction of specific heat capacity based on [17]. For interrupted cooling, this transition is towards the heating curve, and in the case of interrupted heating, the transition moves to a curve lying between the heating and cooling curves [23]. This method has proven effective for this specific task, but the authors themselves recommend a deeper exploration of the topic and validation of the model through experiments [19].

Ivshin and Pence [21] laid the theoretical foundation for the curve-scale modelling approach, which utilises scaled-down heating or cooling enthalpy curves for interrupted solidification and melting processes, respectively. This approach is very similar to the above-mentioned work by Delcroix et al. [19]; however, the transition is not piece-wise linear but rather smooth (depending on the definition of the heating and cooling curves). Subsequent to its inception, this approach has garnered widespread adoption within the scientific community, with numerous scholars achieving notable precision in their analyses. Significant contributions include the works of Thonon [22] and Barz [4, 16, 27], among others, who have all demonstrated the efficacy of this modelling technique, further solidifying its reputation as a robust framework for elucidating complex phase transition behaviour.

Models relying on instantaneous toggling, especially the isoenthalpic (proposed by Rose et al. [20]) and isothermal (introduced by Dentel and Stephan [18]) transitions, are considered rather unreliable and unsuitable for partial phase change modelling. This is because such transitions might violate energy conservation laws, resulting in an over-estimation or underestimation of the latent heat absorbed or released during the phase transition [19].

2.1.4. Inverse problem

Identification of the heating and cooling effective heat capacity curves, which govern the thermal behaviour during the phase change, is a rather difficult task. Many authors opted for experimental measurement methods such as DSC or T-history and simply used the measured data to construct the two-curve model [5, 6, 10, 13, 14]. However, this may pose a problem as these measurement methods only represent the properties of a small sample. In many cases, the obtained enthalpy/effective heat capacity curves cannot be directly applied in the numerical model without significant inaccuracies [13, 28].

2.2. SCOPE OF WORK IN RELATION TO THE CURRENT STATE OF KNOWLEDGE

As an alternative approach, the solution to the IHTPs could be adopted [11]. IHTPs are gaining traction due to their ability to deduce material properties or boundary conditions from the observed temperature fields. This approach involves the formulation of an optimization problem where the goal is to minimize the discrepancy between the observed temperature data and the temperature field predicted by a numerical model. The optimisation algorithm converges towards a solution that best matches the experimental data by iteratively adjusting the parameters of interest, such as the shape of effective heat capacity curves or boundary conditions.

2.2. Scope of work in relation to the current state of knowledge

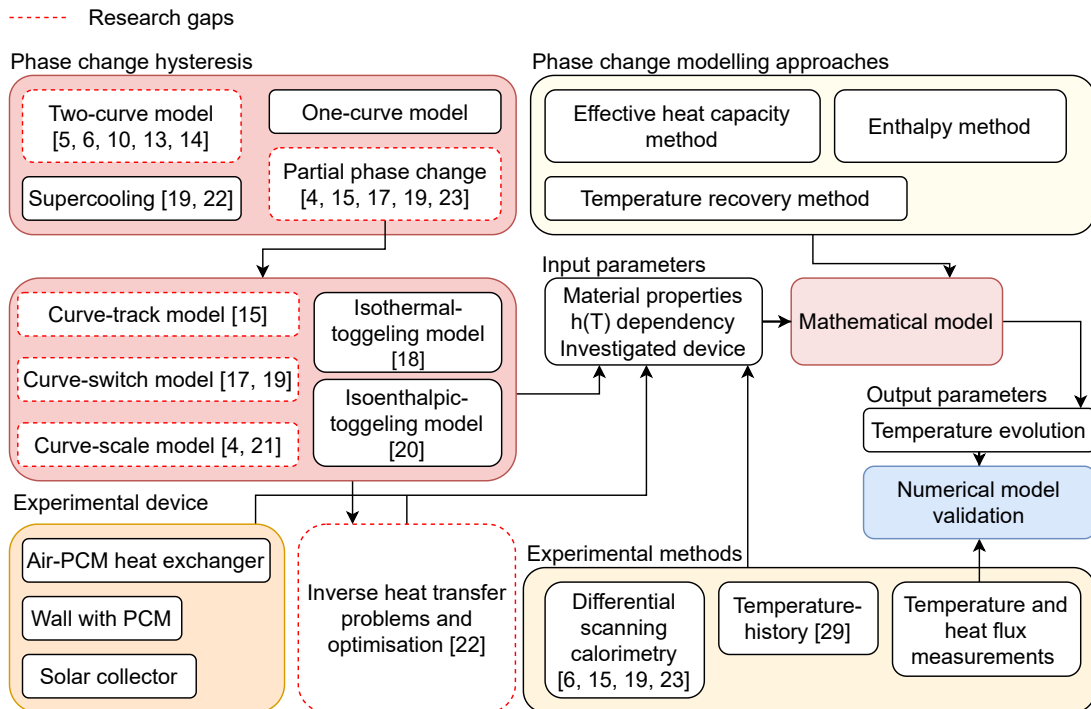


Figure 2.1: The schematic solution of the problem and delineation of research gaps

Based on publications from the state-of-the-art research section, the dissertation thesis proposes a methodology for the identification of thermal behaviour during PCH using inverse problems and optimization methods, addressing a significant research gap in the field (as shown in Figure 2.1). Currently, most authors studying PCM hysteresis utilize well-established models [5, 6, 10, 13, 14, 26], largely based on experimental measurements and the two-curve model. A new perspective on behaviour description was proposed primarily by [4, 19, 22], involving transitions along a curve lying between the heating and cooling curves. The dissertation will focus on a methodology for identifying PCM's thermal behaviour during phase change hysteresis. Furthermore, all of the aforementioned methods still require additional experimental validation, as they are typically validated only on a small sample of data or not at all.

3. AIMS OF THE STUDY

The individual research aims and objectives were specified as results of the mid-term evaluation as

- (A) Description of PCM's thermal behaviour during the phase change hysteresis (PCH) phenomenon. Development of the PCH numerical model using the modelling approaches obtained during the literature review and experimental data measured with the differential scanning calorimetry (DSC) or temperature history (T history) method.
- (B) Development of a parametric model of enthalpy-temperature dependency during the PCH.
- (C) Investigation of thermal behaviour of PCMs during PCH with the use of inverse problems and optimisation.

3.1. Scientific questions and hypotheses

Scientific question 1:

- *“In what manner can the thermal hysteresis of materials during partial phase transitions be qualitatively described? How can these qualitative relationships be transformed into the form of a computer model that enables the solution of temperature distribution in materials during such partial phase changes?”*

The working hypothesis, which serves as the fundamental means in seeking an answer to the aforementioned scientific question, is as follows:

- From the current macroscopic perspective on the issue, capturing hysteresis is suitable through the enthalpy-temperature or effective heat capacity-temperature dependence. However, curves for paired changes (e.g., melting and solidification) are shifted in temperature. Experimental study of partial changes allows the determination of these curves. Transitions between hysteresis curves in the enthalpy-temperature dependence during partial phase transformations have a significant impact on the temperature evolution in PCMs [23]. The differential scanning calorimetry (DSC) method is the most common tool for describing hysteric behaviour [6, 15, 19, 23], but it characterizes only a small amount of material. An alternative is the T-history method, which can describe the behaviour of a larger amount of PCM [29]. Transitions will be realized between hysteresis curves for melting and solidification, which will be determined for complete phase transformation. It is appropriate to conduct these transitions in the direction of specific heat capacity [17, 19, 23] in

the case of interrupted solidification. For interrupted melting, a transition occurs to a curve lying between the melting and solidification curves [19]. Current state-of-the-art research points towards the curve-scale model as the most suitable for partial phase changes. However, for more complex behaviour (random cycling around the phase change temperature), it is necessary to appropriately combine or modify these approaches since none of the current methods adequately describes this phenomenon by itself.

Scientific question 2:

- “How to parameterize the dependence of specific heat capacity (or enthalpy) on temperature to best capture the hysteric behaviour of PCMs? In what manner could the values of the necessary parameters for these curves be identified?”

Working hypothesis:

- The basis for parameterisation will involve numerical methods for phase change modelling, specifically the effective heat capacity method and the enthalpy method. In the first step, a numerical model will be implemented for the specific studied device. Using the numerical model along with experimentally measured temperature profiles in specific locations of the studied PCM, an inverse problem will be designed to identify the effective heat capacity function or the enthalpy dependence on temperature. This will be achieved through heuristic optimization methods. The complexity of the task will significantly depend on the parameterisation of the mentioned functional dependencies, the type of hysteresis model, and the temperature profile in the PCM itself.

3.2. Thesis layout

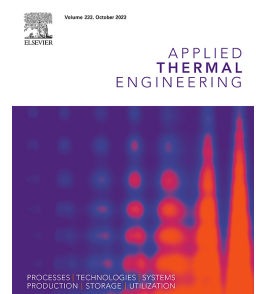
The aim and objectives have been addressed in five stand-alone peer-review journal papers. The number of citations taken from Scopus as of June 2024:

[I.] ZÁLEŠÁK, Martin, Pavel CHARVÁT and Lubomír KLIMEŠ. Identification of the effective heat capacity–temperature relationship and the phase change hysteresis in PCMs by means of an inverse heat transfer problem solved with metaheuristic methods. *Applied Thermal Engineering* [online]. 2021, vol. 197, pp. 117392. ISSN 1359-4311. Available from: doi:<https://doi.org/10.1016/j.applthermaleng.2021.117392>.

Journal impact factor = 6.4, Quartile Q1 (THERMODYNAMICS; ENGINEERING, MECHANICAL and MECHANICS)

Citations: 19

Author’s contribution: 33 %

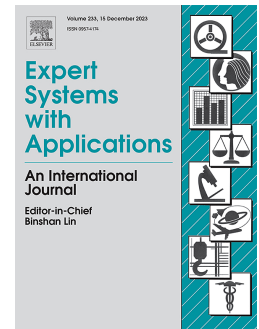


[II.] KŮDELA, Jakub, **Martin ZÁLEŠÁK**, Pavel CHARVÁT, Lubomír KLIMEŠ and Tomáš MAUDER. Assessment of the performance of metaheuristic methods used for the inverse identification of effective heat capacity of phase change materials. *Expert Systems with Applications* [online]. 2024, vol. **238**, pp. 122373. ISSN 0957-4174. Available from: doi:<https://doi.org/10.1016/j.eswa.2023.122373>.

Journal impact factor = 8.5, Quartile Q1 (COMPUTER SCIENCE, ARTIFICIAL INTELLIGENCE; ENGINEERING, ELECTRICAL & ELECTRONIC; OPERATIONS RESEARCH & MANAGEMENT SCIENCE)

Citations: 4

Author's contribution: 40 % (The first and second authors each contributed 40%).

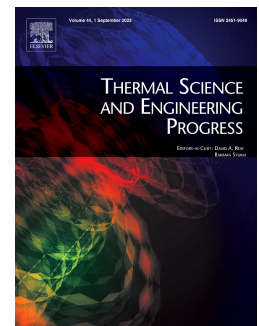


[III.] **ZÁLEŠÁK, Martin**, Pavel CHARVÁT, Lubomír KLIMEŠ, KŮDELA, Jakub and PECH Ondřej. Inverse identification of thermal behaviour of PCMs during complete and partial melting-to-solidification cycles. *Thermal Science and Engineering Progress*. 2024. Article status is currently Under Review. Manuscript number: TSEP-D-24-00657.

Journal impact factor = 4.8, Quartile Q1 (THERMODYNAMICS; ENGINEERING, MECHANICAL; MECHANICS)

Citations: 0

Author's contribution: 60 %



[IV.] **ZÁLEŠÁK, Martin**, Lubomír KLIMEŠ, Pavel CHARVÁT, Matouš CABALKA, Jakub KŮDELA and Tomáš MAUDER. Solution approaches to inverse heat transfer problems with and without phase changes: A state-of-the-art review. *Energy* [online]. 2023, vol. **278**, pp. 127974. ISSN 0360-5442. Available from: doi:<https://doi.org/10.1016/j.energy.2023.127974>.

Journal impact factor = 8.9, Quartile Q1 (THERMODYNAMICS; ENERGY & FUELS)

Citations: 9

Author's contribution: 35 %



[V.] Tomáš MAUDER, Jakub KŮDELA, Lubomír KLIMEŠ, **Martin ZÁLEŠÁK** and Pavel CHARVÁT. Soft computing methods in the solution of an inverse heat transfer problem with phase change: A comparative study. *Engineering Applications of Artificial Intelligence*. 2024, vol. **133**, pp. 108229. ISSN 0952-1976. Available from: doi:<https://doi.org/10.1016/j.engappai.2024.108229>.

Journal impact factor = 8, Quartile Q1 (AUTOMATION & CONTROL SYSTEMS; COMPUTER SCIENCE, ARTIFICIAL INTELLIGENCE; ENGINEERING, ELECTRICAL & ELECTRONIC; ENGINEERING, MULTIDISCIPLINARY)

Citations: 0

Author's contribution: 15 %



4. SUMMARY OF CONDUCTED WORK

4.1. Paper [I.] (Research goals (A) and (C))

Research paper titled *Identification of the effective heat capacity–temperature relationship and the phase change hysteresis in PCMs by means of an inverse heat transfer problem solved with metaheuristic methods* focused on the application of metaheuristic optimization algorithms to the inverse identification of the relationships between the effective heat capacity and temperature during melting and solidification of PCMs. The study developed a procedure for the identification of the effective heat capacity–temperature dependency from the inverse heat transfer problem and tested it on an air-PCM heat exchanger as a heat transfer problem with phase change. The experimental validation of the proposed solution procedure for the inverse problem involved two sets of experimentally derived boundary conditions, referred to as cases A and B. Case A was previously explored in a study conducted by the authors [30], where an air-PCM heat exchanger consisting of 100 compact storage module (CSM) panels was investigated. For case B, the boundary conditions were obtained using a slightly modified version of the air-PCM heat exchanger employed in the aforementioned study [30].

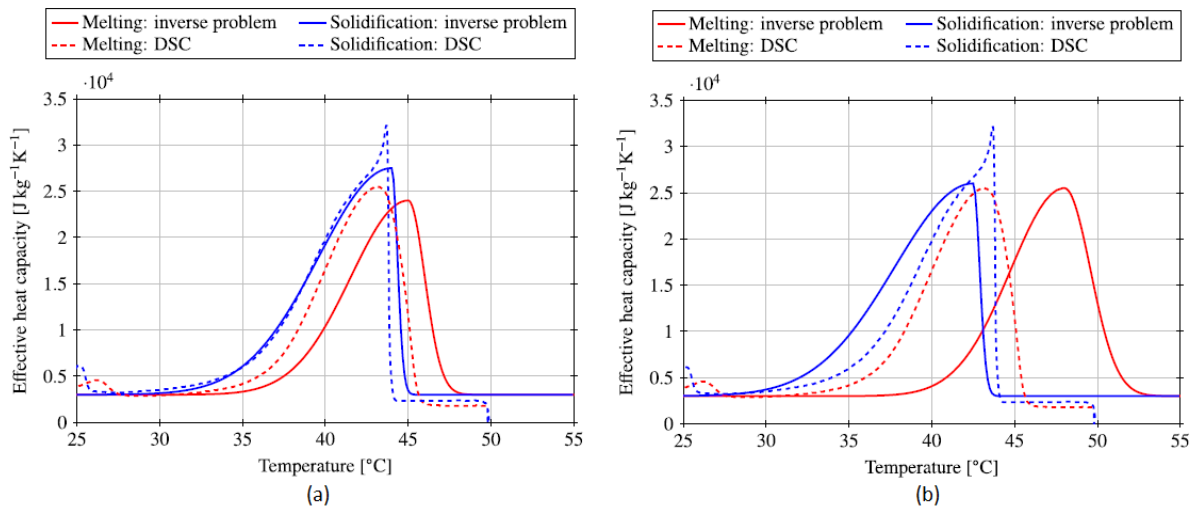


Figure 4.1: Effective heat capacity curves obtained as a solution to the IHTP (a) for case A and (b) case B

The research utilised a two-curve model with phase change hysteresis for the phase change description, assuming the relationship between the effective heat capacity and

4.2. PAPER [II.] (RESEARCH GOALS (B) AND (C))

temperature during melting and solidification of the PCM in the form of two asymmetric Gaussian curves. Each curve is defined by four independent parameters (c , c_{L_f} , T_{ppc} , σ), expressed by the following equation

$$c_{\text{eff}}(T) = c + c_{L_f} \exp \left\{ \frac{(T - T_{\text{ppc}})^2}{\sigma} \right\}, \quad (4.1)$$

where T_{ppc} stands for the peak temperature of the phase change, c is the specific heat capacity in solid/liquid phase outside the phase change temperature range, c_{L_f} is the height coefficient representing the amount of phase change enthalpy, and the sharpness coefficient σ , defined as

$$\sigma = \begin{cases} \sigma_s & \text{for } T \leq T_{\text{ppc}} \\ \sigma_\ell & \text{for } T > T_{\text{ppc}}, \end{cases} \quad (4.2)$$

represents the sharpness and asymmetry of the $c_{\text{eff}}(T)$ function, where σ_s and σ_ℓ is the sharpness in the solid phase and liquid phase, respectively.

Summary of main findings

The study demonstrated the accuracy of the developed procedure when tested on pre-simulated data, achieving less than 3 percent error when assessing the phase change enthalpies. The average temperature difference (error) between the pre-simulated and inversely identified outlet air temperature at a time instant was $2.55 \cdot 10^3$ K and $1.66 \cdot 10^3$ K for the particle swarm optimisation (PSO) and differential evolution (DE) methods, respectively. However, the accuracy decreased when the procedure was applied to data obtained by lab-scale experiments, with the average temperature error between the experimentally obtained and inversely identified outlet air temperatures at a time instant ranging from 0.032 to 0.039 K, depending on the considered experimental dataset. The most significant discrepancy, observed at the end of the solidification processes, was likely a result of neglecting the secondary phase transitions in the simulation model.

Furthermore, the discrepancy between the phase change enthalpies obtained by the DSC and those obtained by the solution of the inverse problem ranged from 2.9% to 15.7%. Additionally, the temperatures of the phase change peaks, identified from the inverse problem, differed by between 0.34 °C and 4.93 °C from the temperatures obtained from the DSC analysis as shown in Figure 4.1.

4.2. Paper [II.] (Research goals (B) and (C))

Research paper titled *Assessment of the performance of metaheuristic methods used for the inverse identification of effective heat capacity of phase change materials* proposes an inverse identification procedure which utilises heuristic optimization methods to solve the inverse problem of determining the effective heat capacity of PCMs with focus on an air-PCM heat exchanger unit as the investigated device. Contrary to the research paper [I.], this paper does not discuss the PCH and focuses on the solution to the IHTPs and parametrisation of the effective heat capacity curve. The mathematical model of the heat exchanger unit was used to simulate the thermal behaviour of the PCM and generate pre-simulated (synthetic) data as substitutes for experimental measurements (a similar approach was also partially adopted in the research paper [I.]). The article compares

the performance of seven different metaheuristic methods for the inverse identification procedure applied to the total of 5 different cases. The initial three case studies were developed with pre-simulated outlet air temperatures using the specified set of input parameters as shown in Figure 4.2. This ensured the condition $OF(\mathbf{p}) = OF(\mathbf{p}_{pre-sim}) = 0$, where \mathbf{p} is the vector of optimisation variables. The effective heat capacity curves corresponding to the chosen parameters are depicted in Figure 4.2. All three scenarios maintained symmetry with respect to the specific heat capacity in the solid and liquid states ($c_\ell = c_s$).

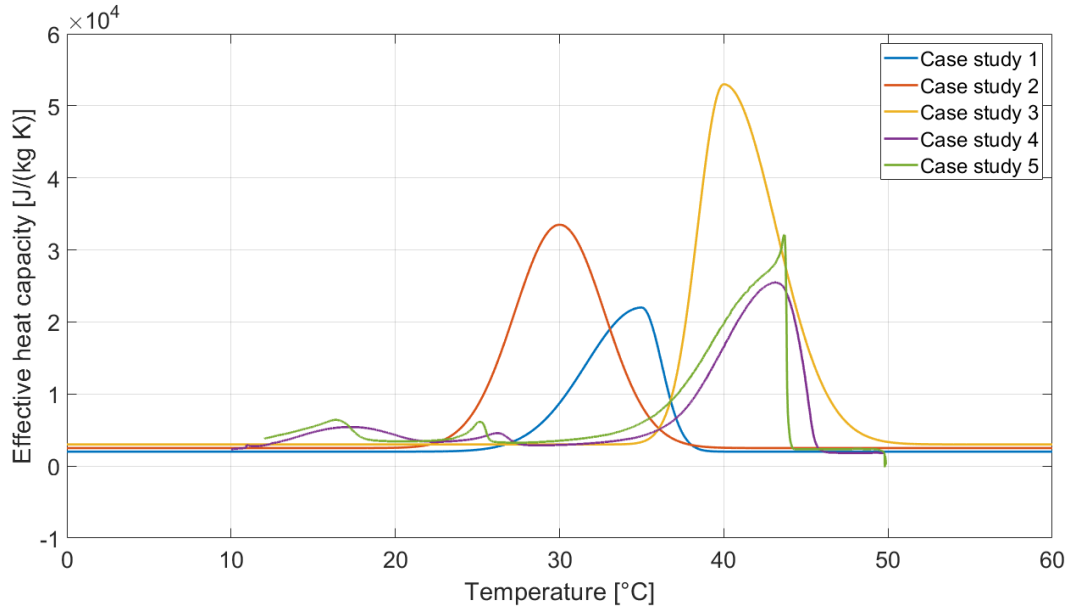


Figure 4.2: Pre-simulated (synthetic) effective heat capacity curves

For case studies 4 and 5, pre-simulated data were generated using the heating and cooling effective heat capacity curves obtained from DSC measurements for an organic paraffin-based PCM (Rubitherm RT42). In these instances, it is ensured that $\nexists \mathbf{p} \in M : OF(\mathbf{p}) = 0$, where M represents the set of feasible solutions specified in the paper. This is due to multiple peaks and various spikes contained in the effective heat capacity curves from the DSC measurement.

Summary of main findings

In the comparative study, seven different heuristic optimization methods were analyzed. The methods included success-history based adaptive differential evolution with linear population size reduction (LSHADE), DE (Differential evolution), PSO (Particle swarm optimization), CMA-ES (Covariance matrix adaptation evolution strategy), TLBO (Teaching-learning based optimization), CS (Cuckoo search), and ABC (Artificial bee colony). The two best-performing metaheuristic methods were LSHADE and DE. LSHADE performed the best when higher computational resources were available and provided results with better precision when compared to the other methods. On the other hand, DE was more suitable when lower precision was required, and computational resources were limited. For the first three case studies, the best found solutions perfectly identified the input parameters. However, for case studies 4 and 5, the best found solutions of the extended model had average squared errors of $1.768E-02 \text{ } ^\circ\text{C}^2$ and $6.158E-03 \text{ } ^\circ\text{C}^2$, respectively. This

4.3. PAPER [III.] (RESEARCH GOALS (A), (B), AND (C))

is due to the much more complex nature of case studies 4 and 5, as the temperature evolution was calculated with experimental effective heat capacities obtained by DSC measurement.

The study employed the effective heat capacity method for phase change modeling, utilizing an asymmetrical Gaussian function as the chosen parametrisation. Therefore, the effective heat capacity function was defined as

$$c_{\text{eff}}(T) = \begin{cases} c_s + (c_M - c_s) \exp \left\{ \frac{(T-T_{\text{ppc}})^2}{\sigma_s} \right\} & \text{for } T \leq T_{\text{ppc}}, \\ c_\ell + (c_M - c_\ell) \exp \left\{ \frac{(T-T_{\text{ppc}})^2}{\sigma_\ell} \right\} & \text{for } T > T_{\text{ppc}}, \end{cases} \quad (4.3)$$

where $c_M = c_{L_f} + c_s$ represents the peak value of the c_{eff} function, T_{ppc} is the peak phase change temperature, σ_s and σ_ℓ describe the sharpness of the Gaussian function and c_s and c_ℓ are heat capacities in the solid and liquid states, respectively.

The investigation exclusively focused on an approach involving a singular effective heat capacity curve, thereby disregarding the PCH. The asymmetry of the curve is attributed to both the shape within the phase change region, formed by the connection of two distinct Gaussian functions at their peaks, and by the distinction of the specific heat capacity in the solid and liquid phases. The comparative analysis underscored the critical role of appropriately parameterising the effective heat capacity curve in the inverse identification procedure. It was demonstrated that enhancing the accuracy of results is achievable by introducing distinct specific heat capacity values for the solid and liquid states.

4.3. Paper [III.] (Research goals (A), (B), and (C))

The research paper titled *Inverse identification of thermal behaviour of a paraffin-based phase change material in complete and partial phase change cycles* focused on solving the IHTPs with PCMs during complete and partial melting-to-solidification cycles. This paper could be considered the core of this thesis as it deals with all three research goals (A), (B), and (C). The study involved the construction and validation of a numerical model for complete and partial phase changes, as well as an assessment of different partial phase change models. It contains a novel parameterisation approach to effective heat capacity-temperature relationship based on a two-piece normal distribution (TPND). The research also utilised an inverse heat transfer problem to obtain effective heat capacity curves for different cases, specifically focusing on the curve-scale, curve-switch, and curve-track models.

Summary of main findings

The study delved into the nuances of phase change hysteresis and the importance of accurately modelling PCMs for various applications, particularly in thermal energy storage systems. The methodology involved the development of a numerical model using the control volume method in conjunction with the effective heat capacity approach to describe the thermal behaviour accurately. The experimental setup included a paraffin-based PCM Rubitherm RT35HC, and the manufacturer-provided effective heat capacity curves were utilised for validation. To induce both melting and solidification of the PCM, the experimental setup incorporated Peltier cells, which were capable of generating the required heat flux. A total of 9 Peltier cells were strategically positioned in a uniform 3 by 3 distribution within an additively manufactured socket grid, and they were placed between

4.3. PAPER [III.] (RESEARCH GOALS (A), (B), AND (C))

an aluminium plate and a passive cooler. This arrangement enabled control over the heat flux applied to the PCM sample, allowing for the simulation of complete and interrupted melting-to-solidification cycles. Temperature monitoring within the experimental setup was facilitated by the use of PT100 sensors, which were strategically positioned to capture temperature variations at critical locations. The entire experimental setup was enclosed in thermal insulation to minimise heat loss and to maintain the integrity of the experimental conditions.

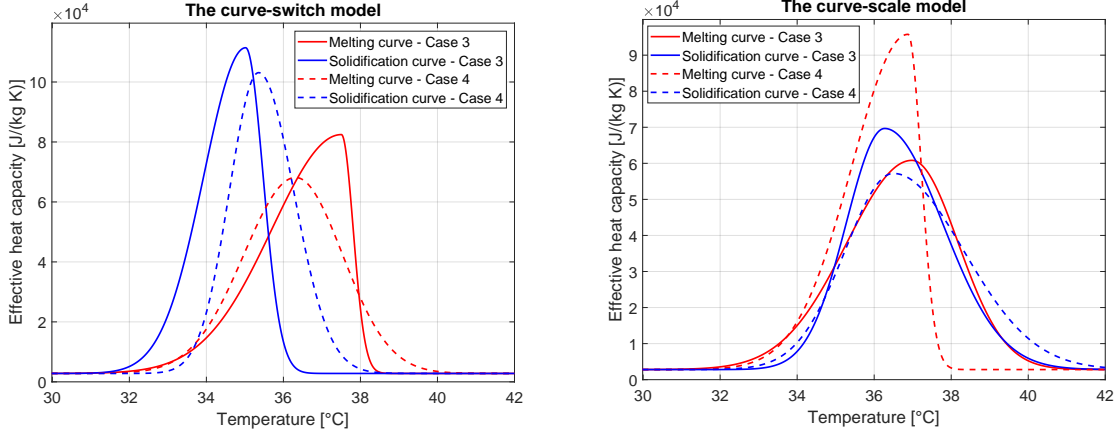


Figure 4.3: Results to an IHTP: Case 3 and Case 4

The effective heat capacity function was conceptualised as an asymmetric Gaussian function. In this context, an analogy with a TPNP can be applied, using a formulation adapted from [31, 32] as

$$c_{\text{eff}}(T) = \begin{cases} c_s + (c_l - c_s)\xi(T) + A \exp \left\{ \frac{-(T-T_{\text{peak}})^2}{2\sigma_s^2} \right\} & \text{for } T \leq T_{\text{peak}}, \\ c_s + (c_l - c_s)\xi(T) + A \exp \left\{ \frac{-(T-T_{\text{peak}})^2}{2\sigma_l^2} \right\} & \text{for } T > T_{\text{peak}}, \end{cases} \quad (4.4)$$

where $A = L_f \sqrt{\frac{2}{\pi}} (\sigma_l + \sigma_s)^{-1}$ is a scaling factor, L_f is the enthalpy of fusion, $\xi \in [0,1]$ represents the liquid fraction of PCM, c_s and c_l is the specific heat capacity in the solid and liquid state, respectively, T is the temperature, T_{peak} denoted a peak phase change temperature, and σ_s and σ_l is a skewness parameter for the solid and liquid state, respectively.

The research also involved comparing different modelling approaches, such as the curve-switch, curve-scale, and curve-track transition-based modelling approaches, to examine partial phase changes. For complete phase changes, both straightforward one-curve and two-curve models were assessed and compared with the effective heat capacity curves provided by the manufacturer.

The accuracy of the different modelling approaches was evaluated, with the curve-scale model consistently demonstrating superior performance in both cases 3 and 4 for partial phase changes. The RMSE values for the curve-scale model were reduced by 60% and 99% for cases 3 and 4, respectively, compared to the manufacturer's data. For complete phase changes, the two-curve approach exhibited the highest level of accuracy, showcasing a substantial improvement in RMSE of up to 62% when compared to the manufacturer's data. The study also notes that the curve-track model demonstrated the least accuracy among the three models under consideration for partial phase changes.

4.4. Paper [IV.] (Research goal (C))

Research paper titled *Solution approaches to inverse heat transfer problems with and without phase changes: A state-of-the-art review* provides a comprehensive review of various methods and approaches for solving inverse heat transfer problems (IHTPs) with and without phase changes. The review covers a wide range of solution methods, including conventional iterative methods, meta-heuristic algorithms, fuzzy logic, and data-driven methods such as artificial neural networks (ANNs) and machine learning (ML). Despite being a review article, it has been incorporated into the dissertation thesis because it addresses one of the scientific questions formulated in Chapter 3.1, in particular Scientific question 2 (“*How to parameterise the dependence of specific heat capacity (or enthalpy) on temperature to best capture the hysteric behaviour of PCMs? In what manner could the values of the necessary parameters for these curves be identified?*”).

Summary of main findings

The review emphasises the challenges associated with solving IHTPs, including non-linearity, multi-modality, high dimensionality, and the lack of detailed physical descriptions of the phenomena. These challenges underscore the need for robust and versatile solution methods capable of addressing complex and intricate problems. The results indicate that incorporating regularization techniques enables traditional methods to counteract the detrimental effects of noise within the data, potentially enhancing solution stability and yielding improved outcomes. Nonetheless, effectively choosing optimal regularization parameters poses a daunting task, requiring careful consideration of the balance between solution accuracy and smoothness during the process. On the other hand, the meta-heuristic methods proved as highly adaptable and efficient optimization tools, often offering a universal solution for problems of diverse complexity. These methods employ stochastic search algorithms, which explore the search space with greater efficacy compared to conventional gradient-based methods, thus introducing randomness into the search process. Meta-heuristic methods have demonstrated increased robustness and effectiveness, especially in the pursuit of global optima, when contrasted with conventional approaches. However, it’s important to note that the solution yielded by meta-heuristic methods doesn’t inherently guarantee the attainment of the global optimum.

The literature has limited insights into the practical application of ANNs and fuzzy logic in this field due to the significant need for input data. This knowledge gap underscores the necessity for further exploration to thoroughly assess the use of ANNs and fuzzy logic in processes involving heat and mass transfer, both with and without phase changes. The literature review reveals a lack of information on evaluating and comparing different methods for solving heat and mass transfer problems. To address this research gap, a thorough comparative study covering various complexities of heat and mass transfer processes and utilizing a wide range of solution methods would be valuable. Additionally, the paper emphasises the importance of expert knowledge and experience in selecting appropriate solution methods for specific heat and mass transfer processes.

4.5. Paper [V.] (Research goal (C))

Research paper titled *Soft computing methods in the solution of an inverse heat transfer problem with phase change: A comparative study* diverges from the other research papers within this thesis by addressing the inverse identification of boundary heat flux. In contrast to papers that concentrate on effective heat capacity curves, this research primarily focuses on the determination of boundary conditions, with the aim of achieving the research goal (C). The modelling approach dealing with the direct heat transfer problem (HTP) was based on 1D heat conduction, as shown in Figure 4.4. An inverse identification framework, applicable to problems both with and without phase change, was established in this study. It offers an investigation of versatile boundary conditions or material properties, such as effective heat capacity or enthalpy. Four distinct methods, rooted in diverse mathematical principles (see Figure 4.5), are employed and comprehensively compared. The methods encompass a conventional Levenberg-Marquardt method (LMM), a predictive fuzzy logic (PFL)-based approach, a population-based meta-heuristic method named LSHADE (an advanced variant of differential evolution), and a newly devised surrogate-assisted method combined with differential evolution, denoted as the LSADE method.

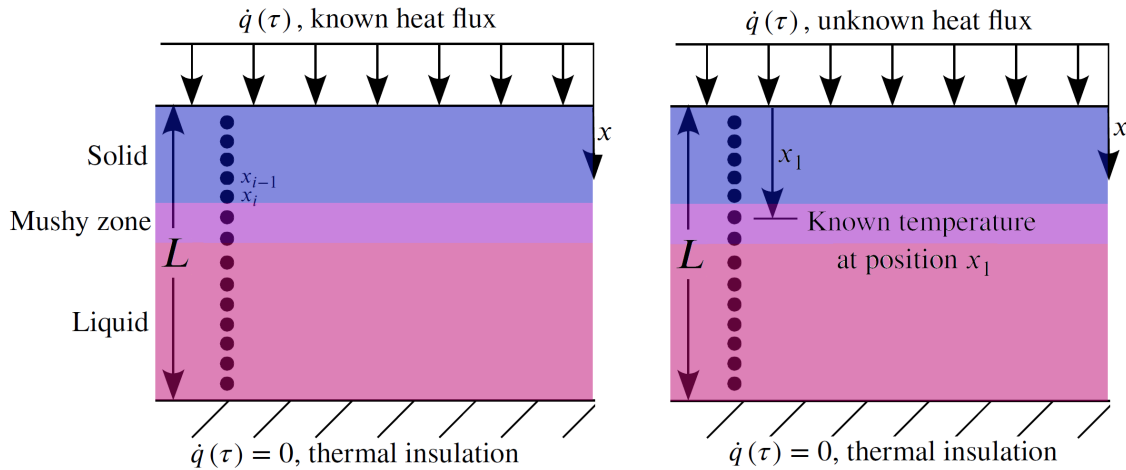


Figure 4.4: Illustration of direct and inverse problems: On the left, a direct problem is depicted where a known boundary heat flux is given, and the goal is to determine the temperature distribution. On the right, an inverse problem is presented where the temperature at a specified location, x_1 , is known, and the objective is to determine the boundary heat flux.

Summary of main findings

The study evaluated various methods for solving inverse heat transfer problems with and without phase change. Conventional methods like the LMM and the PFL method performed well in linear problems without phase change but significantly deteriorated when phase change was introduced. Conversely, meta-heuristic-based methods like LSHADE and surrogate-assisted LSADE performed consistently well in both scenarios, significantly outperforming LMM and PFL. LSHADE and LSADE methods demonstrated stability and low sensitivity to temperature sensor location, making them superior choices. In contrast, LMM and PFL methods heavily relied on sensor proximity to achieve acceptable solutions, showing significant performance drops with increasing distance. Furthermore, the

LSHADE and LSADE methods were identified as suitable for boundary heat flux inverse problems with phase change, while LMM and PFL were deemed inappropriate due to their low performance. However, implementing LSHADE and LSADE methods was noted to be challenging compared to LMM and PFL, which might still serve as viable options for problems not involving phase change and with sensors located near the surface.

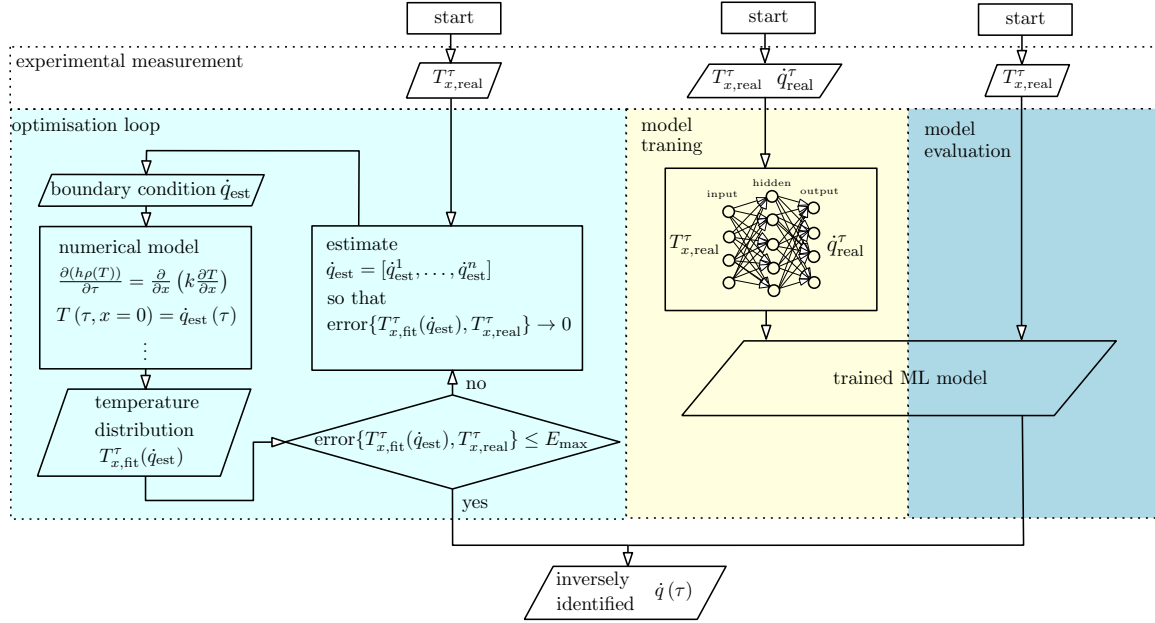


Figure 4.5: Physics-based and data-driven solution methods to IHTPs

CONCLUSIONS

This thesis explored the thermal behaviour of phase change materials (PCMs) undergoing phase change hysteresis (PCH) through numerical and experimental methods. An inverse identification framework was developed based on solutions to inverse heat transfer problems (IHTPs), and potential methods for parameterising effective heat capacity curves were introduced. The key findings address the scientific gaps outlined in Chapter 3:

- In most computer models that incorporate PCH, two separate enthalpy-temperature, effective heat capacity-temperature, or liquid fraction-temperature curves for melting and solidification are commonly employed. Therefore, all modelling methodologies adopt a macroscopic perspective rooted in fundamental thermodynamic principles (e.g. effective heat capacity method, enthalpy method). The transition between these curves, if present, serves as the defining factor for the PCH modelling approach.
- The complete phase changes can be accurately modelled using the two-curve approach. However, caution is needed when using melting and solidification curves from experimental techniques like DSC or temperature-history methods [13]. These methods assume uniform temperatures across the PCM sample, which may not reflect real-world conditions in latent heat thermal energy storage systems. Additionally, they are limited by small sample sizes and are affected by the chosen heating/cooling rate. Investigations based on IHTPs are better suited for specific problems.
- The modelling of partial phase change cycles presents a considerably more intricate and challenging task, demanding the toggling between the melting and solidification curves or the incorporation of transition modelling within the temperature range of phase change. The results of this thesis indicate the superior performance of the curve-scale modelling approach, closely followed by the curve-switch modelling approach. In contrast, the curve-track model demonstrated the least favourable performance and is therefore deemed unsuitable for modelling partial phase changes. These findings align with previous research on partial phase transitions, supported by a body of literature, including references such as [16, 19, 22, 23].
- Meta-heuristic methods, known for their versatility and efficiency, often outperform conventional optimization techniques by effectively exploring the search space through stochastic processes. Unlike traditional gradient-based methods like the Levenberg–Marquardt method (LMM) or Beck’s sequential function specification method, meta-heuristics are more robust and adept at finding global optima. Recent studies highlight the effectiveness of the differential evolution (DE) method and its variants, especially those with success-history based parameter adaptation

and linear population size reduction schemes, such as LSHADE [33, 34]. Although the particle swarm optimization (PSO) method converges more slowly, it remains a reliable solution for addressing IHTPs [35].

- The thesis highlights the importance of using the right parameterisation for the effective heat capacity curve in the inverse identification process. It shows that incorporating different specific heat capacities for solid and liquid states improves model accuracy.

Engineers designing latent heat thermal energy storage (LHTES) systems can gain valuable insights from this thesis. It provides an understanding of the PCH phenomenon and models both complete and partial phase change cycles and introduces a framework for the inverse identification of material properties and boundary conditions.

4.6. Future research

Various techniques have been proposed for modelling phase change hysteresis in partial phase change cycles; however, their validation remains relatively incomplete. Validation efforts have been confined to specific configurations and materials within only a limited extent. To establish the overall applicability of the proposed methods, there is a substantial need for comprehensive research that spans a wide range of cases and operational conditions. This would contribute to a more thorough understanding and confirmation of the effectiveness of these methods across various scenarios.

While a substantial body of research focuses on solving IHTPs using conventional and meta-heuristic methods, fewer studies explore artificial neural networks (ANNs), machine learning (ML), and fuzzy logic for this purpose. Further investigation is needed to assess the applicability and efficiency of these methods for IHTPs. Advanced ML approaches, such as physics-informed neural networks (PINNs), supervised machine learning, convolutional neural networks, generative adversarial networks, automated ML, and recurrent neural networks, also hold promise for IHTP solutions. However, the current knowledge of these advanced methods in the context of IHTPs is limited, highlighting the need for more research.

4.7. Limitations

The research outlined in this thesis focused on organic paraffin-based PCMs (in particular manufactured by Rubitherm from the RT product series). It is essential to exercise caution when extrapolating and applying the findings to different PCMs, such as salt hydrates, which can experience PCH with the peak temperature shift of up to several degrees Celsius [12]. Furthermore, multi-step transitions could significantly widen the temperature spectrum. For instance, this phenomenon has been observed in fatty acid esters and paraffins [16], where it arises from a solid-solid latent phase transition at lower temperatures preceding the solid-liquid transition at higher temperatures. The transitional behaviour during partial phase changes might be influenced by the increasing peak temperature shift, and other phenomena, such as supercooling, could interfere with the PCH behaviour. Most of the authors also reported that PCH might be influenced by the heating/cooling rate applied to the PCM sample.

References

- [1] AL-SAAD, Saleh Nasser and Zhiqiang ZHAI. Modeling phase change materials embedded in building enclosure: A review. *Renewable and Sustainable Energy Reviews*. 2013, vol. 21, pp. 659–673.
- [2] LIN, Wenye, Zhenjun MA, Haoshan REN, Stefan GSCHWANDER and Shugang WANG. Multi-objective optimisation of thermal energy storage using phase change materials for solar air systems. *Renewable Energy*. 2019, vol. 130, pp. 1116–1129.
- [3] CABEZA, Luisa F and Harald MEHLING. *Review on Phase changing materials to store energy* [online]. 2003. ISBN 3497370274. Available from: doi:10.1016/S1359-4311(02)00192-8.
- [4] BARZ, Tilman and Andreas SOMMER. Modeling hysteresis in the phase transition of industrial-grade solid/liquid PCM for thermal energy storages. *International Journal of Heat and Mass Transfer*. 2018, vol. 127, pp. 701–713.
- [5] GOIA, Francesco, Gaurav CHAUDHARY and Stefano FANTUCCI. Modelling and experimental validation of an algorithm for simulation of hysteresis effects in phase change materials for building components. *Energy and Buildings*. 2018, vol. 174, pp. 54–67.
- [6] MORELES, Efraín, Guadalupe HUELSZ and Guillermo BARRIOS. Hysteresis effects on the thermal performance of building envelope PCM-walls. *Building Simulation*. 2018, vol. 11, pp. 519–531.
- [7] GOWREESUNKER, B. L. and S. A. TASSOU. Effectiveness of CFD simulation for the performance prediction of phase change building boards in the thermal environment control of indoor spaces. *Building and Environment*. 2013, vol. 59, pp. 612–625.
- [8] CABEZA, L.F., I. MARTORELL, L. MIRĂŁ, A.I. FERNĂÑDEZ and C. BARRENECHÉ. 1 - Introduction to thermal energy storage (TES) systems. 2015, pp. 1–28.
- [9] KLIMEŠ, Lubomír, Pavel CHARVÁT, Mahmood MASTANI JOYBARI, Martin ZÁLEŠÁK, Fariborz HAGHIGHAT, Karthik PANCHABIKESAN, Mohamed EL MANKIBI and Yanping YUAN. Computer modelling and experimental investigation of phase change hysteresis of PCMs: The state-of-the-art review. *Applied Energy*. 2020, vol. 263, pp. 114572.
- [10] BISWAS, Kaushik, Yash SHUKLA, Andre DESJARLAIS and Rajan RAWAL. Thermal characterization of full-scale PCM products and numerical simulations, including hysteresis, to evaluate energy impacts in an envelope application. *Applied Thermal Engineering*. 2018, vol. 138, pp. 501–512.

- [11] ZÁLEŠÁK, Martin, Lubomír KLIMEŠ, Pavel CHARVÁT, Matouš CABALKA, Jakub KŮDELA and Tomáš MAUDER. Solution approaches to inverse heat transfer problems with and without phase changes: A state-of-the-art review. *Energy*. 2023, vol. 278, pp. 127974.
- [12] JIN, Xing, Huoyan HU, Xing SHI and Xiaosong ZHANG. Energy asymmetry in melting and solidifying processes of PCM. *Energy Conversion and Management*. 2015, vol. 106, pp. 608–614.
- [13] STATHOPOULOS, N., M. EL MANKIBI and Mattheos SANTAMOURIS. Numerical calibration and experimental validation of a PCM-Air heat exchanger model. *Applied Thermal Engineering*. 2017, vol. 114, pp. 1064–1072.
- [14] KUZNIK, F. and J. VIRGONE. Experimental investigation of wallboard containing phase change material: Data for validation of numerical modeling. *Energy and Buildings*. 2009, vol. 41, pp. 561–570.
- [15] CHANDRASEKHARAN, Ramprasad, Edwin S LEE, Daniel E FISHER and Pratik S DEOKAR. An Enhanced Simulation Model for Building. 2013, pp. 1–11.
- [16] BARZ, Tilman. Paraffins as phase change material in a compact plate-fin heat exchanger Part II: Validation of the “curve scale” hysteresis model for incomplete phase transitions. *JOURNAL OF ENERGY STORAGE*. 2021, vol. 34.
- [17] BONY, Jacques and Stéphane CITHERLET. Numerical model and experimental validation of heat storage with phase change materials. *Energy and Buildings*. 2007, vol. 39, pp. 1065–1072.
- [18] DENTEL, A and W STEPHAN. TRNSYS TYPE 399-Phase change materials in passive and active wall constructions. *Institute for Energy and Building, Georg Simon Ohm University of Applied Sciences: Nürnberg, Germany*. 2013.
- [19] DELCROIX, Benoit, Michaël KUMMERT and Ahmed DAOUD. Development and numerical validation of a new model for walls with phase change materials implemented in TRNSYS. *Journal of Building Performance Simulation*. 2017, vol. 10, pp. 422–437.
- [20] ROSE, Jørgen, Andreas LAHME, Niels Uhre CHRISTENSEN, Per HEISELBERG, Magne HANSEN and Karl GRAU. Numerical method for calculating latent heat storage in constructions containing phase change material. *IBPSA 2009 - International Building Performance Simulation Association 2009*. 2009, pp. 400–407.
- [21] IVSHIN, Yefim and Thomas J. PENCE. A constitutive model for hysteretic phase transition behavior. *International Journal of Engineering Science*. 1994, vol. 32, pp. 681–704.
- [22] THONON, Maxime, Gilles FRAISSE, Laurent ZALEWSKI and Mickael PAILHA. Analytical modelling of PCM supercooling including recalescence for complete and partial heating/cooling cycles. *Applied Thermal Engineering*. 2021, vol. 190, pp. 116751.
- [23] DELCROIX, Benoit, Michaël KUMMERT and Ahmed DAOUD. Thermal behavior mapping of a phase change material between the heating and cooling enthalpy-temperature curves. *Energy Procedia*. 2015, vol. 78, pp. 225–230.
- [24] MUHIEDDINE, Mohamad, É CANOT and R MARCH. Various approaches for solving problems in heat conduction with phase change. *International Journal on Finite Volumes*. 2009, vol. 6, pp. 66–85.

- [25] JIN, Xing, Xiaodong XU, Xiaosong ZHANG and Yonggao YIN. Determination of the PCM melting temperature range using DSC. *Thermochimica Acta*. 2014, vol. 595, pp. 17–21.
- [26] DOLADO, Pablo, Ana LAZARO, Jose M. MARIN and Belen ZALBA. Characterization of melting and solidification in a real-scale PCM-air heat exchanger: Experimental results and empirical model. *Renewable Energy*. 2011, vol. 36, pp. 2906–2917.
- [27] BARZ, Tilman, Adam BURUZS and Andreas SOMMER. Major and minor hysteresis loops in the enthalpy-temperature and phase fraction-temperature diagrams of solid/liquid phase change materials. *International Journal of Engineering Science*. 2023, vol. 191.
- [28] ALVAREZ-RODRIGUEZ, Matias, Mar ALONSO-MARTINEZ, Ines SUAREZ-RAMON and Paulino JOSÉ GARCÍA-NIETO. Numerical model for determining the effective heat capacity of macroencapsulated PCM for building applications. *Applied Thermal Engineering*. 2024, vol. 242, pp. 122478.
- [29] MARÍN, José M., Belén ZALBA, Luisa F. CABEZA and Harald MEHLING. Determination of enthalpy-temperature curves of phase change materials with the temperature-history method: Improvement to temperature dependent properties. *Measurement Science and Technology*. 2003, vol. 14, pp. 184–189.
- [30] CHARVÁT, Pavel, Lubomír KLIMEŠ and Milan OSTRÝ. Numerical and experimental investigation of a PCM-based thermal storage unit for solar air systems. *Energy and Buildings*. 2014, vol. 68, pp. 488–497.
- [31] WALLIS, Kenneth F. The Two-Piece Normal, Binormal, or Double Gaussian Distribution: Its Origin and Rediscoveries. *Statistical Science*. 2014, vol. 29, pp. 106–112.
- [32] VILLANI, Mattias and Rolf LARSSON. The Multivariate Split Normal Distribution and Asymmetric Principal Components Analysis. *Communication in Statistics-Theory and Methods*. 2005, vol. 35.
- [33] KŮDELA, Jakub, Martin ZÁLEŠÁK, Pavel CHARVÁT, Lubomír KLIMEŠ and Tomáš MAUDER. Assessment of the performance of metaheuristic methods used for the inverse identification of effective heat capacity of phase change materials. *Expert Systems with Applications*. 2024, vol. 238, pp. 122373.
- [34] MAUDER, Tomáš, Jakub KŮDELA, Lubomír KLIMEŠ, Martin ZÁLEŠÁK and Pavel CHARVÁT. Soft computing methods in the solution of an inverse heat transfer problem with phase change: A comparative study. *Engineering Applications of Artificial Intelligence*. 2024, vol. 133, pp. 108229.
- [35] ZÁLEŠÁK, Martin, Pavel CHARVÁT and Lubomír KLIMEŠ. Identification of the effective heat capacity–temperature relationship and the phase change hysteresis in PCMs by means of an inverse heat transfer problem solved with metaheuristic methods. *Applied Thermal Engineering*. 2021, vol. 197, pp. 117392.
- [36] CHARVÁT, Pavel, Lubomír KLIMEŠ and Martin ZÁLEŠÁK. 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*. 2019, vol. 12.

- [37] ZÁLEŠÁK, Martin, Pavel CHARVÁT and Lubomír KLIMEŠ. Robustness and Accuracy of the Particle Swarm Optimisation Method in the Solution of Inverse Heat Transfer Problems with Phase Change. *Chemical Engineering Transactions*. 2021, vol. 88, pp. 301–306.
- [38] ZÁLEŠÁK, Martin, Lubomír KLIMEŠ and Pavel CHARVÁT. Design Optimization of a Solar Air Collector Integrating a Phase Change Material. *Chemical Engineering Transactions*. 2020, vol. 81, pp. 211–216.
- [39] ZÁLEŠÁK, Martin, Lubomír KLIMEŠ and Pavel CHARVÁT. Design Optimization of a Solar Air Collector Integrating a Phase Change Material. *Chemical Engineering Transactions*. 2020, vol. 81, pp. 211–216.
- [40] KLIMEŠ, Lubomír, Petr KAMARÝT, Pavel CHARVÁT, Martin ZÁLEŠÁK and Martin PEŠEK. Solution to Inverse Heat Transfer Problems by Means of Soft Computing Approach and Its Comparison to the Well-Established Beck's Method. *Chemical Engineering Transactions*. 2022, vol. 94, pp. 433–438.
- [41] ZÁLEŠÁK, Martin, Lubomír KLIMEŠ, Pavel CHARVÁT, Ondřej PECH and Patrik BOUCHAL. An Effective Thermal Conductivity-based Approach for Modelling of Convective Heat Transfer in a Rectangular Cavity Filled with PCM. *Chemical Engineering Transactions*. 2023, vol. 103, pp. 715–720.
- [42] ZÁLEŠÁK, Martin, Pavel CHARVÁT, Lubomír KLIMEŠ and Jirí DUDA. Assessment of Modelling Approaches for Partial Phase Changes of PCMs. *Chemical Engineering Transactions*. 2022, vol. 94, pp. 457–462.
- [43] ZÁLEŠÁK, MARTIN, BOUCHAL, PATRIK, OSTRÝ, MILAN and HEJČÍK, JIŘÍ. Experimental set up for the investigation of partial phase changes of phase change materials. *EPJ Web Conf.* 2022, vol. 264, pp. 01049.
- [44] ZÁLEŠÁK, Martin, Pavel CHARVÁT and Lubomír KLIMEŠ. Robustness and Accuracy of the Particle Swarm Optimisation Method in the Solution of Inverse Heat Transfer Problems with Phase Change. *Chemical Engineering Transactions*. 2021, vol. 88, pp. 301–306.
- [45] KLIMEŠ, Lubomír, Jakub KŮDELA, Martin ZÁLEŠÁK and Pavel CHARVÁT. *A Solution to an Inverse Heat Transfer Problem With Phase Change by Means of Meta-Heuristics and Artificial Neural Networks: A Comparative Study* [online]. 2023. Available from: <https://doi.org/10.1115/IMECE2023-113333>. Available from: doi:10.1115/IMECE2023-113333.
- [46] ZÁLEŠÁK, Martin, Pavel CHARVÁT, Lubomír KLIMEŠ, Ondřej PECH and Patrik BOUCHAL. *Thermal Behavior of PCMs During Phase Transitions With Phase Change Hysteresis: Experimental Setup Development and Problems of Model Validation* [online]. 2023. Available from: <https://doi.org/10.1115/IMECE2023-113269>. Available from: doi:10.1115/IMECE2023-113269.
- [47] ZÁLEŠÁK, Martin, Pavel CHARVÁT, Lubomír KLIMEŠ, Jakub KŮDELA and Ondřej PECH. Inverse identification of thermal behaviour of a paraffin-based phase change material in complete and partial phase change cycles. *Thermal Science and Engineering Progress*. 2024, vol. 51, pp. 102585.

MARTIN ZÁLEŠÁK

Mathematical Engineer / Software Engineer

@ martin.zal7@gmail.com Brno, Czech Republic in www.linkedin.com/in/mzalesak/
www.orcid.org/0000-0001-6697-2644



EDUCATION

PhD. in Energetics

Brno University of Technology

📅 Sep 2018 – June 2024 Brno, Czech Republic

Ing. in Mathematical Engineering

Brno University of Technology

📅 Sep 2016 – May 2018 Brno, Czech Republic

Bc. in Mathematical Engineering

Brno University of Technology

📅 Sep 2013 – May 2016 Brno, Czech Republic

EXPERIENCE

PhD. Student

Brno University of Technology

📅 Sep 2018 - Present Brno, Czech Republic

- Thesis title: Inverse identification of hysteresis behaviour of paraffin-based phase change materials.
- Main areas of the study: numerical modelling, optimization, thermal behaviour of PCM.
- PCMs are mostly utilised in thermal energy storage systems.

Systems Engineer Intern

Thermofisher Scientific

📅 Sep 2018 - Dec 2019 Brno, Czech Republic

- Work focused on the development of the Helios 5 electron microscope.
- The main focus: the optimization of objective lenses by taking into account the electromagnetic hysteresis phenomena.
- Engineering work combined with scripting in Python. Working with autoscript/XT toolkit libraries.
- The main outcome was the optimal profile of the Degauss function.

Mathematical Engineer Junior

4dot

📅 June 2018 - Sep 2018 Brno, Czech Republic

- Working on the software used for an analysis of the industrial machines.
- Software was developed in Python/MATLAB using the Fourier analysis and deconvolution.

Experimental Technician

Heat Transfer and Fluid Flow Laboratory

📅 June 2016 - Sep 2016 Brno, Czech Republic

- Experimental work on metal cooling technologies.
- Temperature measurements and data analysis.

TECHNICAL STRENGTH

Python
MATLAB
L^AT_EX



STRENGTHS

Hard-working

Problem solving

Mathematics

Optimization

Python

Thermomechanics

LANGUAGES

English
German



PUBLICATIONS

- Author or co-author of 7 journal papers (5 of those in the first quartile by JCR) and 10 conference papers.
- H-index: 5 (Scopus), 4 (WoS)
- Scopus citations (excluding self-citations) > 98

ABSTRACT

From the macroscopic point of view, phase change hysteresis (PCH) signifies that the trajectory of a phase change process (e.g., solidification) doesn't mirror the temperature-enthalpy pathway of its inverse process (melting). Despite being a prevalent phenomenon in most phase change materials (PCMs), it tends to be overlooked in computational models, leading to disparities when compared with experimental data. PCH becomes particularly problematic in the modelling of latent heat thermal energy storage systems, where incomplete or partial phase transitions are frequently encountered. Laboratory-scale techniques for PCM characterisation, such as differential scanning calorimetry or the temperature-history method, often employ only small PCM samples, and the resultant data may prove inadequate for predicting the thermal dynamics of larger PCM volumes. In this thesis, the state-of-the-art modelling approaches to PCH were investigated and implemented in the form of a mathematical model. The two-curve model (in its general implementation) was adopted with good accuracy for complete phase changes. However, its applicability falls short in scenarios where the phase transition process is interrupted. The curve-track, curve-switch, and curve-scale models were investigated for partial phase changes. Among these, the curve-scale model emerges as the most precise, aligning with the state-of-the-art analysis. On the other hand, the curve-track model exhibits the least accuracy and is deemed inadequate for partial phase transitions. The presented inverse identification framework, grounded in solving inverse heat transfer problems (IHTPs), proved effective in identifying a diverse array of input parameters. However, the primary emphasis lies in identifying the effective heat capacity curves and their associated parameters. These curves were parameterised using an asymmetrical Gaussian function, incorporating differing specific heat capacities for the solid and liquid segments and dividing each curve into two Gaussian functions separated by the phase change temperature, with skewness introduced for each segment. The thesis demonstrated that this asymmetry resulted in a closer alignment with experimental data. Meta-heuristic optimization techniques were found to be robust and precise in addressing IHTPs, with the differential evolution (DE) method and its variants, particularly the success-history based adaptive differential evolution with linear population size reduction (LSHADE), demonstrating superior performance compared to other meta-heuristics.

ABSTRAKT

Z makroskopického hlediska znamená hystereze změny skupenství (PCH - z angl. phase change hysteresis), že trajektorie procesu fázové změny (například tuhnutí) nezachycuje teplotně-entalpickou cestu svého inverzního procesu (tání). Přestože je to běžný jev u většiny materiálů pro fázovou změnu (PCMs - z angl. phase change materials), často se přehlíží v počítačových modelech, což vede k rozdílům ve srovnání s experimentálními daty. PCH se stává zvláště problematickou při modelování systémů pro ukládání tepelné energie, kde často dochází k neúplné nebo částečné fázové přeměně. Laboratorní přístupy k charakterizaci PCM, jako je diferenciální skenovací kalorimetrie nebo metoda teplotní historie, umožňují studium pouze malých vzorků PCM a výsledná data se mohou ukázat jako nedostatečná pro predikci tepelné dynamiky větších objemů PCM. V této práci byly zkoumány a implementovány moderní přístupy k modelování PCH ve formě matematického modelu. Pro úplné fázové změny byl použit dvoukřivkový model s dobrou přesností, nicméně jeho základní varianta selhává v situacích, kde je proces přechodu fáze přerušen. Dále byly zkoumány modely curve-track, curve-switch a curve-scale pro částečné fázové změny. Mezi nimi se model curve-scale jeví jako nejpřesnější a v souladu se současným stavem poznání v této oblasti. Na druhou stranu model curve-track vykazuje nejmenší přesnost a je považován za nevhodný pro částečné fázové přeměny. Představený framework pro inverzní identifikaci, založený na řešení inverzních problémů přenosu tepla (IHTPs - z angl. inverse heat transfer problems), se ukázal jako velmi účinný při identifikaci různých vstupních parametrů. Primární důraz byl však kladen na identifikaci křivek efektivní tepelné kapacity a s nimi souvisejících parametrů. Tyto křivky byly parametrizovány pomocí asymetrické gaussovské funkce, která zahrnovala různé měrné tepelné kapacity pro pevnou a kapalnou část a každou křivku rozdělila do dvou gaussovských funkcí oddělených teplotou fázové změny, přičemž byla zavedena šikmost pro každý z těchto segmentů. Práce ukázala, že tato asymetrie vedla k lepší shodě s experimentálními daty. Bylo zjištěno, že metaheuristické optimalizační techniky jsou robustní a přesné při řešení IHTPs, přičemž metoda diferenciální evoluce a její varianty, zejména metoda založená na historii úspěchu adaptivní diferenciální evoluce s lineárním snižováním velikosti populace (LSHADE), prokázaly lepší přesnost ve srovnání s jinými metaheuristikami.