

Article

Multizone Modeling for Hybrid Thermal Energy Storage

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Abstract: This study presents a one-dimensional mathematical model developed to simulate multi-zone thermal storage systems using phase change materials (PCMs). The model enables precise analysis of temperature distribution in the layered storage based on several PCM configurations and properties. It is distinguished by its adaptability to various tank geometries and the number of PCM capsules, enabling its application under diverse operating conditions. By simplifying the implementation of heat transfer processes that depend on the shape of the capsule and the thermal properties of the PCM, the computation time can be reduced to a level that makes simulations over longer periods feasible. Experimental validation confirmed the accuracy of the model, with deviations below 6%, underscoring its practical applicability. The study demonstrates that individual layering in the storage tank can be achieved by filling it with PCMs of different melting points without compromising the maximum storage capacity. It is shown that including a PCM layer can maintain the outlet temperature 20% longer while storing 14% more energy. The results point out the model's potential to improve the performance of thermal storage systems through targeted PCM layer configurations. The model serves as the basis for the planning and optimization of these systems.

Keywords: phase change material; energy storage; numerical simulation; latent heat; packed beds



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1. Introduction

To address climate change, reducing total energy consumption and transitioning to renewable energy usage are both crucial. Optimizing storage systems presents a significant opportunity, since renewable energies are not always consistently available. Efficiently storing renewable energy is essential for making the heating sector more sustainable. In this context, thermal energy storage systems, especially those utilizing phase change materials (PCMs), offer a flexible solution for heat storage [1]. PCM energy storage systems are employed in various applications, often in solar heating and cooling systems [2], and for improving thermal comfort in buildings and vehicles [3,4]. The advantage of PCMs lies in their ability to store and release energy during phase transitions, which is particularly useful for enabling nearly constant temperature heat absorption or emission. These systems exhibit increased energy density, which can save space. In this context, packed bed latent heat storage systems have attracted considerable interest due to their extensive heat transfer area between the storage medium and the heat transfer fluid, enabling high loads.

The design of a storage tank and the PCM material are crucial for the performance of hybrid energy storage systems. The tank design must enable optimal stratification and heat transfer to the PCM material to utilize the full capacity of the material at a temperature level suitable for the system. This can mitigate the discrepancy between energy supply and demand during peak load periods [1]. Nallusamy et al. [5] used paraffin in a packed bed to study the impact of porosity and the flow rate of the heat transfer fluid on system performance; the authors concluded that, in addition to improved performance, the PCMs used reduced the volume of the storage tank compared to conventional sensible heat storage tanks. In a study by Sun et al. [6], the thermal properties of latent heat storage in 3-PCM capsules were analyzed using concentric dispersion models, considering radial heat

transfer, wall heat loss, and charging and discharging processes. The effects of porosity, capsule diameter, and the ratio of tank height to diameter on the thermal performance and utilization rates of storage tanks were also examined. It was found that the aspect ratio of the tank did not affect energy storage when the tank volume remained constant. The particle diameter significantly affected the heat transfer between air and PCM capsules in the study; reducing the diameter led to a thinner thermocline and increased energy storage capacity. Teamah et al. [7] found in their study that integrating PCMs into thermal storage systems increases solar utilization at low tank volumes and aligns it with conventional systems at large volumes. The advantages at small volumes result from the lower inlet temperature of the collector fluid, which extends the pump runtime and thereby improves solar energy uptake and collector efficiency, despite slightly increased heat losses.

Most studies focused on spherical capsules, which have the smallest surface-to-volume ratio, resulting in a very small heat transfer area per volume. In their review, Regin et al. [8] found that most studies focused on spherical and cylindrical capsules. However, Grabo et al. [9] examined capsules with a super-ellipsoidal shape and additional grooves and holes, as well as other nonspherical capsule geometries, which increase the packing density of the bed and thus its storage capacity.

The different capsule shapes and sizes, as well as the porosity and permeability of the PCM, influence thermal diffusivity processes. The flow conditions in these complex and finely structured media are difficult to represent, but are essential for the effectiveness of energy storage systems. The complex model of Hariti et al. enables the precise prediction of permeability and porosity in porous media, which is crucial for latent energy storage and other engineering applications [10].

The properties of PCMs to possess low thermal conductivity create a central problem in the use of PCMs in energy storage systems. To improve this, conductive nanoparticles are mixed into the PCM to increase the thermal conductivity of the PCM material. Studies have shown that by blending hybrid nanoparticles, such as 1% Cu and 4% Al_2O_3 , thermal efficiency can be increased and economic benefits can be achieved [11]. Taking into account and carefully selecting suitable materials, their hygroscopic properties and corrosion and hazard levels, as well as thermal and atmospheric stability and costs, the integration of highly conductive additives can improve thermal diffusivity processes and increase the efficiency of thermal latent heat storage [12].

Numerical simulation is a powerful tool for estimating the thermal performance of PCM energy storage systems. Computational fluid dynamics (CFD) is suitable for simulating complex shapes and detailed processes for developing new concepts for PCM energy storage. In an article by Jaffrey et al. [13], an approach for predicting the melting behavior in a packed bed of encapsulated PCM was presented, conducted through detailed simulations of an isolated PCM capsule. The results of these simulations then serve as the basis for a finite-volume model used to predict the total melting time and correct behavior of the PCM temperature throughout a packed bed, which has also been experimentally validated.

Simpler numerical models can be used for system simulations. These simulations help to better understand the dynamic interactions between PCM, heat transfer fluid, the tank, and other components, contributing to improved system efficiency through the precise modeling of heat transfer and storage. A review article by Gracia and Cabeza [14] evaluated numerical methods for analyzing latent heat thermal energy storage systems in packed beds. The models capture simulated fluid flow through porous material without accurately capturing the variations in the cross-sections of the flow channels. The studied models base their accuracy on empirically determined values for the thermal conductivity and heat transfer coefficient of the material. They distinguish between single-phase and two-phase models. Single-phase models consider the solid and liquid phases (here PCM spheres) as a uniform phase, where the temperatures of solid and fluid are instantaneously equated, making them ideal for fixed beds with very high thermal conductivity. In contrast, two-phase models differentiate between solid and liquid phases, with interfaces defined using Nusselt correlations. There are three models: the concentric dispersion model, which

considers thermal conduction in solids; the continuous solid phase model, which views the system as a continuous porous medium; and Schumann's model, which models only convection and heat losses without heat conduction.

Kong and Yang et al. [15] developed a numerical model of a PCM water storage system featuring separate areas for water and PCM, calculated based on common energy conservation equations for both phases. The model includes features such as separate heat loss coefficients and flexible inlets and outlets and was validated through experimental tests covering charging phases, as well as sensible and latent heat discharges, with heat transfer determined from experimental data. The numerical model presented by Papst et al. [16] uses a mushy zone approach to simulate the phase changes of PCMs, capable of depicting the phase transition of a PCM capsule with variable material properties. This simulation of sensible and latent heat transfer has been validated by experiments and lays the foundation for further research on packed beds. This work is based on a combination of advancing Schumann's model by Regin et al. [17] and the previously described approach to depicting phase transitions with variable material data. Regin's model is based on fundamental equations similar to those of Schumann and analyzes the phase change phenomenon of the PCM in the capsules by applying the enthalpy method and a time-dependent overall heat transfer coefficient.

The new aspect of the method in this paper is that it enables the properties of a selected PCM material, along with its thermal characteristics during phase change within the capsule assembly, to be straightforwardly projected in a temperature-dependent manner onto a representative elementary volume without discretizing the PCM capsules.

In summary, integrating phase change materials into thermal energy storage systems presents a promising method for increasing the use of renewable energies while reducing reliance on conventional energy sources.

The aim of this study was to develop a simulation model to represent a thermal latent storage system able to predict the behavior of the storage system with different PCM configurations in terms of the quantity of PCM capsules and varying PCM melting points. Since the energy density of a PCM tank is only slightly higher than that of water, the improvements must be made clear, especially for technical applications. The heterogeneous PCM layers and their influence on forced stratification within a tank are shown.

Another goal was to enable adjustment of the tank geometry. In an extension, the model serves as a basis for optimizing thermal storage systems able to use individual PCM fillings to increase the overall system efficiency through the integration of different heat sources and producers, such as heat pumps and solar heating sources, and consumers.

2. Materials and Methods

2.1. Multizone Storage Tank Model

This mathematical model of the latent heat storage system comprises a separate conservation equation for each zone (water and PCM).

In this setup, the PCM is contained in a heap of nearly cylindrical capsules within the tank and is surrounded by water. The model for the water region can also operate independently of the PCM region, allowing for the analysis of a pure water tank alone. The approach used in this paper for modeling the storage tank is based on a one-dimensional spatial discretization of the energy balance using finite volumes. Figure 1 schematically illustrates the model storage tank. The tank is assumed to be cylindrical. The water and PCM phases are interspersed and interact via a coupled iterative method for their computation. For the required spatial detail accuracy, the storage tank is vertically segmented into a specific number n of horizontal layers, each of the same height. In accordance with the models described in Baeten et al. [18], an energy balance is established for each of these layers. It is assumed that an uneven temperature field in the radial direction due to flow conditions or heat transfer to the tank wall does not occur; thus, a one-dimensional model can adequately represent the tank. As a result, the temperature of the water area and the PCM area within a layer is uniform in the radial direction, and each zone in a layer is in

thermal equilibrium. The first layer is located at the bottom, and the n th layer represents the top layer. The discharge outlet is at the lowest layer of the storage tank, and the loading inlet can be variably placed in a layer between the second and n th layers. The modeling of the phase transition within the PCM capsules from solid to liquid is based on the enthalpy method [16]. Heat convection in the liquid PCM region is not considered in the model.

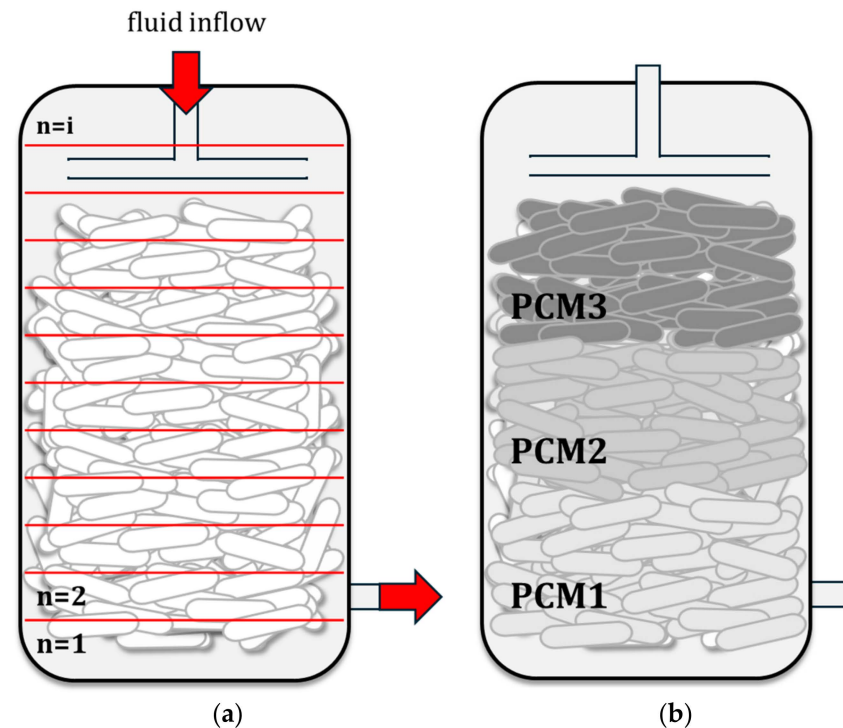


Figure 1. Illustration of the latent heat storage system, divided into n segments (a), PCM sections (b).

Given that the capsules constitute a packed bed configuration within the tank, merely a fraction of the tank's total volume is occupied by water. This fraction is captured by what is known as porosity ε , which represents the ratio of the void volume to the tank volume. The void volume can be calculated by multiplying the number of capsules by their respective volumes and then subtracting this total capsule volume from the tank volume.

$$\varepsilon = \frac{V_T - V_{PCM}}{V_T} \quad (1)$$

To increase flexibility for different tank geometries and the number of PCM capsules, as well as their melting points, the model allows a flexible filling of the tank with PCM capsules. Instead of completely filling the tank with capsules, capsules can be individually placed from the bottom upwards in the tank. Using a porosity known from experiments, an adjusted fill height can then be calculated, which depends on both the number of PCM capsules and the geometry of the storage tank. This approach also allows the modeling of capsules with different melting points in targeted layers within the storage tank. The modeling equations are specified in the following subsections.

2.1.1. Water Zone

During a charging or discharging process, the water zone is an open system in which both energy and matter are exchanged. The differential equation for the water zone of the tank can be formulated for the different layers using Equations (2)–(4).

For the first layer at the tank bottom:

$$\rho c_p A_{ax} \varepsilon \Delta z \frac{dT_1}{dt} = A_{Tank} U_{Tank} (T_{amb} - T_1) + \frac{\lambda_{eff}(A_{ax} - \varepsilon)}{\Delta z} (T_2 - T_1) + \dot{m}_{down} c_p (T_2 - T_1) + \dot{m}_{up} c_p (T_{dis} - T_1) + U_C A_C (T_{PCM\ 1} - T_1) \quad (2)$$

For the middle layer between the bottom layer and the top layer:

$$\rho c_p A_{ax} \varepsilon \Delta z \frac{dT_i}{dt} = A_{Tank} U_{Tank} (T_{amb} - T_i) + \frac{\lambda_{eff}(A_{ax} - \varepsilon)}{\Delta z} (T_{i-1} - 2T_i + T_{i+1}) + \dot{m}_{down} c_p (T_{i+1} - T_i) + \dot{m}_{up} c_p (T_{i-1} - T_i) + U_C A_C (T_{PCM\ i} - T_i) \quad (3)$$

For the last layer N at the tank top:

$$\rho c_p A_{ax} \varepsilon \Delta z \frac{dT_n}{dt} = A_{Tank} U_{Tank} (T_{amb} - T_n) + \frac{\lambda_{eff}(A_{ax} - \varepsilon)}{\Delta z} (T_2 - T_1) + \dot{m}_{down} c_p (T_{ch} - T_n) + \dot{m}_{up} c_p (T_{n-1} - T_n) + U_C A_C (T_{PCM\ n} - T_n) \quad (4)$$

The term on the left side describes the dynamic change in energy of the first layer. A_{ax} represents the base area of the cylindrical volume element. The first term on the right side represents the loss of heat through the tank wall to the surrounding environment. The heat transfer coefficient depends on the flow conditions inside and outside the tank as well as on the material of the tank wall and its insulation. The heat transfer coefficient may vary for each layer n . For properly insulated tanks, this term can be neglected. However, in this work, the storage tank is assumed to be adiabatic. The tank area A_{Tank} for the first and last layers of the storage tank must also include the bottom and top surfaces of the tank, in addition to the lateral surface of the tank. Heat losses or gains are higher at these layers than for the rest of the storage system. The second term on the right side describes the heat conduction between adjacent vertical layers. In real storage systems, due to the good thermal conductivity of the metal container wall, a vertical heat flow through the tank wall affects the surrounding layers and eventually leads to increased mixing within the storage tank [19]. For this purpose, Equation (5), the lambda effective, is introduced, which takes into account the heat conduction through both the water and the tank wall.

The next two terms of Equations (2)–(4) consider the mass flows for charging and discharging. For the layer with the inlet, the temperature during charging corresponds to the charging temperature. The last term describes the energy transferred from the water to the PCM capsules.

$$\lambda_{eff} = \lambda_{Fl} + \lambda_W \frac{A_W}{A_{ax}} \quad (5)$$

The different zones within the thermal energy storage system are defined based on the location and user input for the PCM material and the height of the inlet (top/bottom). The criteria for determining these zones include the type of material (i.e., PCM or water) and the specific elevation within the storage tank at which the inlet is located. If a zone consists exclusively of a water layer, the term for the energy transfer to the PCM layer is omitted. This approach ensures that the model accurately represents the thermal dynamics within the storage system.

2.1.2. PCM Zone

An identical differential equation is established for the PCM domain in Equation (6). There are no heat flows to adjacent layers or the environment, as it is assumed that the PCM capsules only contact the surrounding water and are ideally situated in a single layer. The PCM zone is a closed system.

$$\rho c_p A_{ax} (1 - \varepsilon) \Delta z \frac{dT_i}{dt} = U_C A_C (T_i - T_{PCM\ i}) \quad (6)$$

The heat transfer from the water to the PCM capsule and the heat conduction within the capsule are summarized in the coefficient U_c . This overall heat transfer coefficient is influenced by the specific material properties of the PCM and the capsule material, as well as by the surrounding flow. This coefficient can be calculated through experiments, CFD simulations, or analytical calculations.

Regin et al. [17] employed a resistance model to capture the behavior of a latent heat storage system within a solar water heating system. The model accounts for the conductive resistance layers of the capsule shell and the PCM components by generating an overall heat transfer coefficient (Equation (7)). This coefficient varies depending on the state of the PCM—whether it is fully liquid, fully solid, or passing through the phase change.

$$U_C = \frac{1}{A} \frac{1}{R_{ext} + R_C + R_{in}(t)} \quad (7)$$

Teamah et al. [7] indicated that regardless of the PCM's state—liquid, solid, or mixed—heat transfer within the PCM occurs predominantly through conduction. During the phase transition process, the overall heat transfer coefficient of each capsule's outer surface is calculated by considering the convective thermal resistance at the outer surface of the capsule shell R_{ext} , the conductive resistance through the capsule wall R_C , and the resistance posed by the solid or molten PCM layer within the capsule $R_{in}(t)$. The melting or solidification of the PCM layer is a function of time.

For the model in this study, the resistance model has been adapted. For heat transfer from the capsule shell to the interior of the capsule, a heat conductivity optimized for the geometry and outlined from CFD calculations was presented [16,20]. This conductivity applies to the PCM temperatures inside the capsule below its melting point, considering the heat conductivity of the solid material as a function of a shape factor F_{form} .

$$\lambda = \begin{cases} \lambda_s F_{form} & \text{if } T < T_m \text{ (solid)} \\ \lambda_m F_{form} & \text{if } T = T_m \text{ (melting)} \\ \lambda_l & \text{if } T > T_m \text{ (liquid)} \end{cases} \quad (8)$$

Above the PCM's melting point temperature, the material-specific heat conductivity of the liquid PCM applies. The shape factor F_{form} describes the influence of gravity on the PCM melting time due to the convective components and takes the shape of the PCM capsule into account. Here, $t_{m,zero-g}$ is the time required for the PCM element to melt without gravity and $t_{m,+g}$ is the time for a PCM element under the influence of gravity. The resulting overall heat transfer coefficient is temperature dependent.

$$F_{form} = \frac{t_{m,zero-g}}{t_{m,+g}} \quad (9)$$

The external heat transfer coefficient is calculated based on the flow conditions within the tank. The heat transfer coefficients between a fluid and the particles of a packed bed are greater than those between the fluid and a single particle. According to [21], the following Nusselt correlation determines the heat transfer coefficient:

$$Nu_C = 2 + \sqrt{Nu_{lam}^2 + Nu_{turb}^2} \quad (10)$$

$$Nu_{lam} = 0.664 + \sqrt{Re} \sqrt[3]{Pr} \quad (11)$$

$$Nu_{turb} = \frac{0.037 Re^{0.8} Pr}{1 + 2.443 Re^{-0.1} (Pr^{2/3} - 1)} \quad (12)$$

$$Nu = f_a Nu_C \quad (13)$$

with

$$Nu = \frac{\alpha d_k}{\lambda} \quad (14)$$

$$Re = \frac{u d_k}{\nu \varepsilon} \quad (15)$$

$$Pr = \frac{\nu}{a} \quad (16)$$

The shape factor fa depends on the geometry of the capsule. It is a property of the packed bed and is set at 1.6 for cylindrical segments with a length-to-diameter ratio l/d ranging from 0.24 to 1.2. Here, d_k represents the diameter of a sphere with an equivalent geometric surface area to that of the PCM capsule. The fluid velocity between the capsules plays a crucial role in calculating the Reynolds number. This velocity can be related to the actual fluid velocity within the void spaces, a relationship that is influenced by the porosity, denoted as ε .

To capture the latent energy during phase transitions, the enthalpy method can continue to be used with Equation (17) by utilizing an adjusted specific heat capacity. The enthalpy method has been frequently employed in the literature to describe the behavior of phase change materials, as indicated by Carmona et al. [22]. Here, the enthalpy released during melting or solidification is linearized around the melting point and added to the original specific heat capacity. Within this range around the PCM's melting point, the entire latent heat is released. Based on the current temperature, the fraction of the PCM that has melted can thus be assessed.

$$c_p = \begin{cases} c_{ps} & \text{if } T < T_m \text{ (solid)} \\ c_{pm} + \frac{\Delta h}{\Delta T_m} & \text{if } T = T_m \text{ (melting)} \\ c_{pl} & \text{if } T > T_m \text{ (liquid)} \end{cases} \quad (17)$$

The mixing effect in the water tank results from the thermal instability of the temperatures of the layers. Due to its higher temperature and the resulting lower specific gravity compared to the colder water in the tank, this water rises. The incoming warm water mass additionally causes entrainment of the surrounding water, which extends the mixing zone upwards. In this work, a model of complete mixing is used. If unstable layers are identified at the end of a time step, an average of the water temperatures of these layers is formed, which serves as the final temperature for both layers. This method corresponds to an infinite reverse flow between the layers and is widely used due to its simplicity [15]. These mixings around the storage tank lid can occur due to the locally much larger contact surface with the tank wall, which cools down more strongly than the layers further below. Loading the storage tank below the top layers also leads to these buoyancy effects. The mixing effect is applied only within pure water layers. Within the packed bed, turbulent and natural convection play a role that depends on the capsule shape and porosity and cannot be accurately represented in a one-dimensional model.

2.2. Numerical Iteration Methodology

According to the mathematical model described in the previous chapter, thermal storage is treated in a one-dimensional multi-zone simulation model. The MATLAB R2023b program is used to solve the model equations. Initially, the design of the storage system and the PCM, as well as the operational parameters, are defined. Temperature-dependent physical properties are deposited for both water and PCM. The storage system is divided into N layers, with initial and boundary conditions set for the various layers. For each layer, the water temperature according to Equations (2)–(4) and, if applicable, the PCM temperature according to Equation (6) are calculated iteratively for each time step, coupled through the overall heat transfer coefficient. As soon as the temperatures for water and PCM converge, the next time step is initiated based on the previous one. Using the ode45 solver in MATLAB, the differential equations are solved with adaptive step sizes. When instabilities occur, the time step is reduced. A previously determined maximum time

interval is established based on the flow rate and the smallest cross-sectional area present in the system. This ensures that a particle can be transported from one layer to the next only within this interval.

If temperature inversions occur in layers filled with water at the end of a time step, these layers are mixed. In the one-dimensional model, the temperatures of water and PCM each represent the entire layer. The simulation is terminated according to user-defined parameters, such as time.

3. Experimental Design and Validation

A thermal stratified storage system was experimentally tested. Initially, the storage tank was operated and measured with water, and then filled with PCM material to ensure comparability.

3.1. Experimental Setup

The experimental setup is implemented using a hardware-in-the-loop concept, enabling the setting and measurement of realistic load profiles for a storage system. The main components are two identically sized storage units: one specifically for testing stratifications and the second a combination of latent heat storage with water as the heat transfer fluid. The hardware in the test stand is controlled in an environment specially developed for the test stand using LabVIEW 2018 [23], and measurement data are recorded.

Both tanks have a cylindrical shape with a diameter of 1.2 m, a height of 2 m, and a volume $V = 1.98 \text{ m}^3$. For the hybrid latent heat storage tank, the heat transfer fluid, water, flows through a packed bed with a porosity of $\varepsilon = 0.46$. The charging module of the storage tank is a radial diffuser, which is located below the tank lid and allows good stratification of the water, according to investigations by Findeisen et al. [24,25]. The outlet of the storage tank is at the bottom. Across the height of the storage tank, 10 temperature sensors are evenly distributed. Additionally, on the distributor and consumer sides, there are flow meters as well as additional temperature sensors at relevant points in the system. Figure 2 shows the experimental setup, and the image next to it provides a view into the hybrid latent heat storage tank with the PCM capsules.

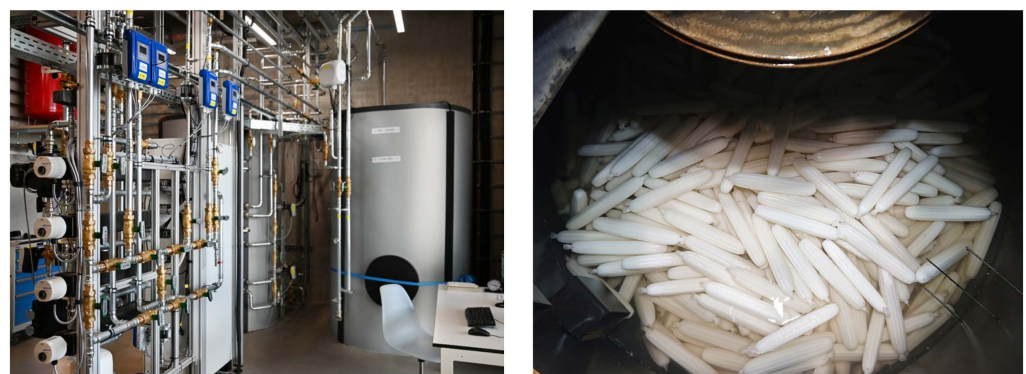


Figure 2. Hardware in the loop test facility (left), latent heat storage tank during filling the packed bed with PCM capsules (right).

Within the tank, there are 1100 capsules filled with CrodaTherm47 (PCM1), and above them are 2400 capsules filled with CrodaTherm60 (PCM2) from CRODA (East Cowick, UK) [26]. The PCM capsules fill the storage tank up to a height of just under 1.6 m. The thermal properties of the PCMs are listed in Table 1. The capsules are produced by Kraft Boxx (Aulendorf, Germany) [27]. The capsule shape resembles a cuboid with a square base of 3.3 cm and a length of 21.5 cm.

Table 1. Material Properties of Crodatherm47 and Crodatherm60.

Material Property	Crodatherm47	Crodatherm60
density [kg/m ³]	940 (solid)/829 (liquid)	922 (solid)/824 (liquid)
specific heat capacity [J/kgK]	1900(solid)/2000 (liquid)	2300 (solid)/1400 (liquid)
thermal conductivity [W/mK]	0.25 (solid)/0.16 (liquid)	0.29 (solid)/0.17 (liquid)
melting temperature [°C]	45 (solid)/47 (liquid)	58 (solid)/60 (liquid)
latent heat [kJ/kg]	210–213	215–219

3.2. Model Validation with Experimental Setup

The simulation was validated using a previous experiment from the test stand described above. In the model, each layer n is assumed to be isothermal, which also implies thermal equilibrium within each layer. This phenomenon is referred to as numerical diffusion in an article by Powell [28]. It results in higher apparent diffusivity in the spatial discretization using the finite difference method for systems with flow than occurs in actual physical mechanisms. The more layers used in the model, the smaller this effect becomes. However, this increases computational time, since more layers require the solving of additional model equations. For areas filled with PCM, these layers theoretically assume that the specified proportion of the PCM is ideally positioned within the layer and behaves isothermally.

Figure 3 shows the impact of the number of layers on the thermocline in a tank with $V = 2 \text{ m}^3$, initially at 30°C , which was charged with water at 70°C at a flow rate of 300 kg/h . The formation of the thermocline after a charging duration of 4 h is shown. The computational times for 10, 100, and 1000 layers in the water storage scenario are 4.3 s, 30.8 s, and approximately 14 min, respectively. On the right side, the same charging scenario is depicted, but the tank contains 3000 PCM capsules with a melting point of 37°C . These 3000 PCM capsules occupy a volume of nearly 0.7 m^3 of the storage tank. Here, the factor by which computational time increases between 100 and 1000 layers is 24. For studies not focusing solely on tank charging, a compromise between precision and computational time should be found to facilitate long-term simulations. Insufficient representation of the thermocline with fewer layers directly affects the amount of water/PCM that stores energy at a sufficiently high temperature.

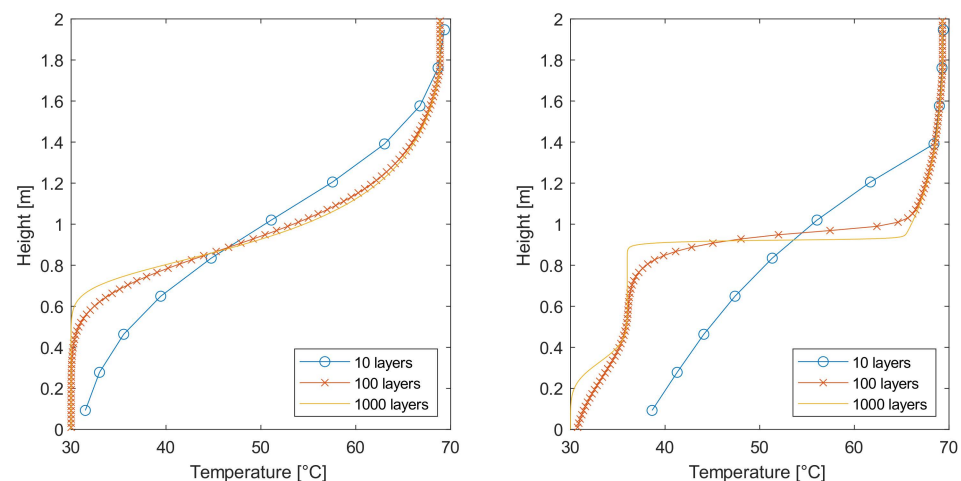


Figure 3. Impact of number of layers on temperature profile in a thermal storage tank with water (**left**) and a thermal storage tank with 3000 capsules of PCM (**right**) with a melting point around 37°C .

Comparing both scenarios here, it becomes evident that the converging solution with many layers for the PCM storage tank can more sharply define the thermocline after 4 h of charging than the solution for the water storage tank.

For the PCM section, it is crucial to ensure that the layer height is chosen to be sufficiently large, as the physical effects due to inadequate model representation of the PCM capsules compared with the experiment are not captured. If the capsules are cut multiple times, there is no energy exchange between the cut surfaces of the PCM capsules. Thus, the division of the layers is tied to the geometry of the capsule in the experiment. If a capsule lies horizontally and thus ideally within a layer, it must be at least 3.4 cm. However, in a random packing, the capsules do not lie ideally in the storage tank and are often slightly inclined. Therefore, a layer thickness of 5.1 cm is calculated, which corresponds to a total of 40 layers. At this value, most PCM capsules are positioned within one layer.

For validation, the measured data were compared with the simulation results. In the experiment, the tank was charged at a loading temperature of 70 °C and a mass flow rate of 300 kg/h. The experiment represents a charging scenario of an empty tank at around 30 °C that is to be completely brought to a temperature level of 60 °C. This does not depict a typical operating scenario of a storage system, but a simple charging process allows for better differentiation of the influences on storage behavior.

For comparison, the temperatures at the 10 temperature measurement points in the tank, distributed over the height of the tank, were compared with the identical points and temperatures of the simulation. The measured values were juxtaposed at the same time after the start of the charging process. The one-dimensional simulation, depicted here in blue, was compared with an experimental trial of the original tank. The measurements show slight variances in the temperature of the charging mass flow over the measurement period, which is constant in the simulation at the aforementioned 70 °C and 300 kg/h. The circular markings correspond to the actual measurement points in the experiment. Figure 4 shows both the measured and simulated temperatures at the entrance and exit of the storage tank. To provide a better overview, the PCM temperature from the simulation of the first layer at the bottom is also displayed. Compared to the simulation, the temperatures at the storage tank inlet were up to 3 K higher than the specified charging temperature. The water temperatures at the outlet align very well up to the 6-h mark, and the PCM capsules also absorb the sensible heat, staying very close to the water temperature. It is not until hour 4 that any influence on the temperature due to the charging process becomes apparent, both in the experiment and the simulation. The temperature gradient changes from hour 4 until reaching the PCM phase change region at 46 °C. Up to the 10-h mark, the PCM temperature remains within the melting range of up to 48 °C, as defined in the simulation. In this range, the water temperatures from the simulation and experiment rise exponentially until reaching 60 °C at the end of the measurement.

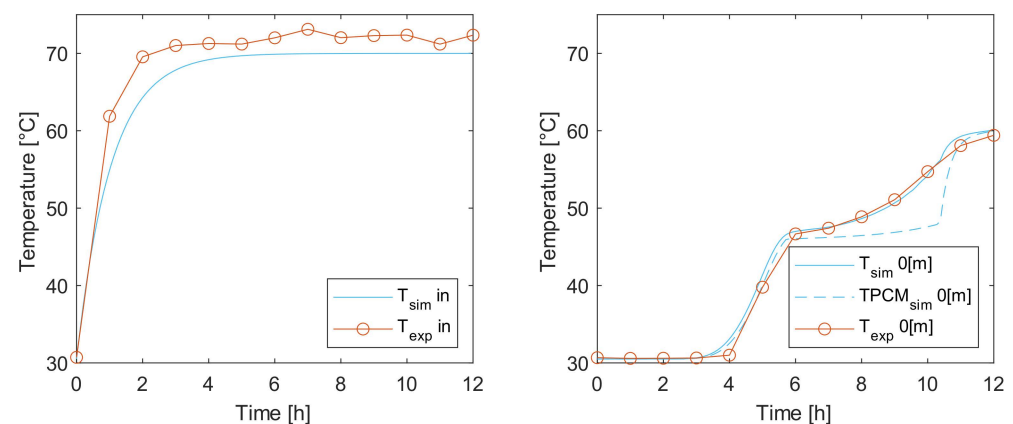


Figure 4. Temperature profile at the inlet and outlet from simulation and experimental data for charging the storage at a temperature of 70 °C and a mass flow rate of 300 kg/h.

As shown in Figure 4, the largest discrepancy between the water temperatures from the experiment and the simulation occurs between the 10th and 11th hours. In the simulation, the temperatures post-phase change are slightly higher, suggesting that the simulation may

not accurately represent the end of the melting process or the transition into the sensible heating phase for the actual capsules. Numerical CFD simulations by Papst [16,20] also suggest that the shape of the capsules used in the experiment could influence this discrepancy. Unlike spherical capsules, cylindrical capsules did not exhibit a clear stagnation of average temperature within the melting range or a gradual increase in temperature in the sensible range.

Figure 5 displays the temperature profiles for various sections of the storage tank. At 1.6 m, just below the radial diffuser, the region contains only the heat transfer fluid, water. At 0.8 m, located in the middle of the PCM2 layer, the melting point is 60 °C. At 0.4 m lies the interface between PCM1 (47 °C) and PCM2 (60 °C). Finally, at 0.2 m, is the PCM1 layer with a melting point at 47 °C. The deviations mentioned are visible here too, shortly after the PCM has finished melting. The discrepancies are most significant near and within the PCM1 layer. However, over time, the temperature difference can be compensated for. No notable deviation is observed in the upper water region apart from the effects of variance in the charging temperature.

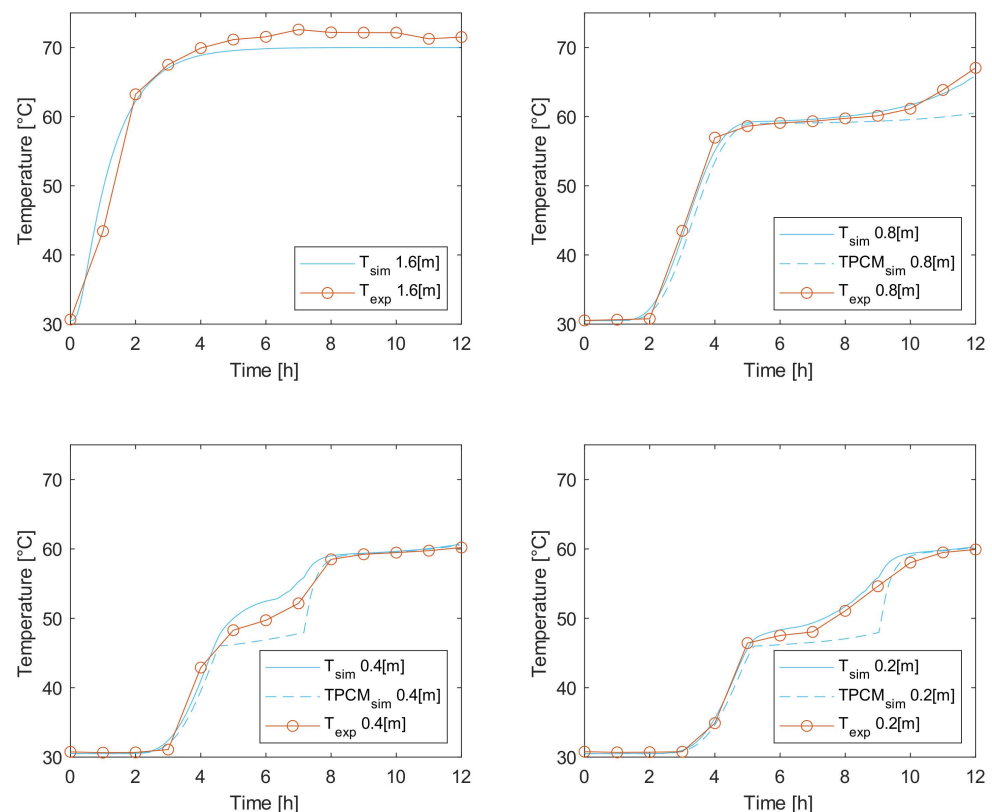


Figure 5. Temperature profiles at various heights in the storage tank, comparing data from simulation and experiment. At the top at 1.6 and 0.8 m, and at the bottom at 0.4 and 0.2 m.

An overall view of the temperature profiles in the storage tank is provided in Figure 6. The overlap of the simulated and experimental data generally shows good agreement. In particular, the slopes of the temperature profiles for each hour are similar. The influence of the PCM melting temperature on the system is also visible for both the experiment and the simulation. Around the melting point of the upper PCM at 60 °C, both curves stagnate similarly until the PCM is theoretically fully melted; only then does the water temperature continue to rise. The same is true for the lower PCM layer. From hour 3 onwards, both in the experiment and simulation, the water temperature enters the melting range of the PCM in the upper area. The PCM with a melting point at 47 °C begins to absorb latent heat around hour 5.

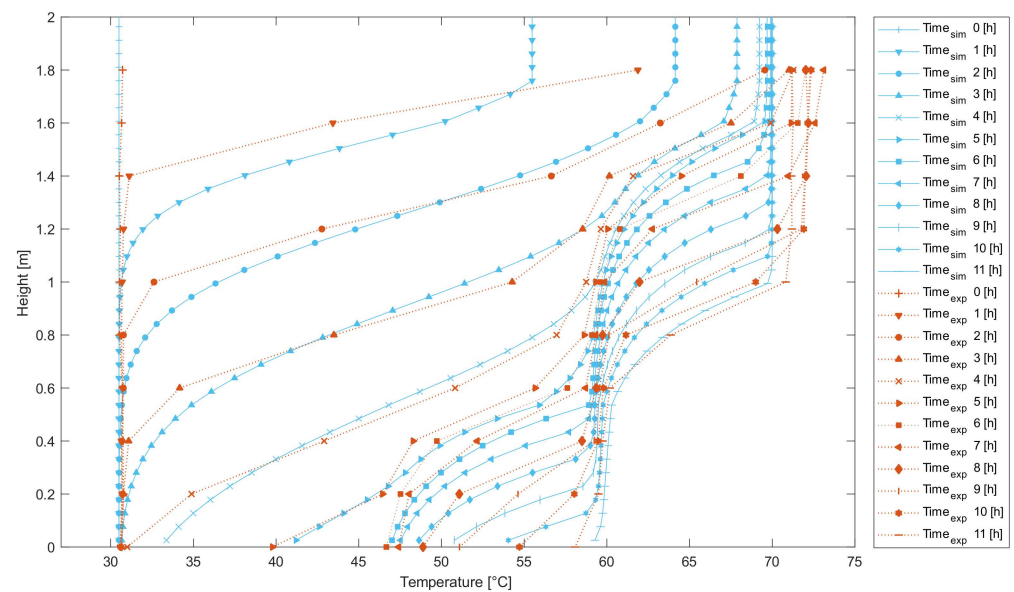


Figure 6. Temperature profiles across the height of the tank over a period of 12 h.

In the latent heat storage tank, thermoclines form in the water, which is disrupted due to the enthalpy uptake at the specific melting point of the PCM. After reaching the melting range for the respective PCM layer, thermocline zones form again on two levels. These shift continuously downward as the charging progresses.

The error between the model and the simulation can be determined using the mean absolute error (MAE) and the mean absolute percentage error (MAPE):

$$\text{MAE}(^{\circ}\text{C}) = \frac{1}{n} \sum_{i=1}^n |E_i - S_i| \quad (18)$$

$$\text{MAPE}(\%) = \frac{1}{n} \sum_{i=1}^n \left| \frac{E_i - S_i}{E_i} \right| \times 100 \quad (19)$$

Using Equation (19), measurements from experiments E_i are compared with the numerical solution S_i at the 10 heights of the measurement points. The simulated PCM storage is calculated using the optimally named layer count of 40 layers. Measurement data and simulation data are taken at the identical times and at the same heights within the storage tank to identify deviations. The model shows a deviation of less than 6% for each layer. The MAE is under 3.2 °C. Compared to the accuracy of the temperature measurements, this is acceptable. The maximum mean absolute percentage error in the hourly comparison of all temperature sensors is below 11%. Thus, the model is declared valid for this technical application area.

In the first column of Table 2, the reference simulation of the experiment can be seen in a parameter comparison. The number of layers is varied, and the respective time step is adjusted. The geometric properties of the tank and PCM correspond to the reference simulation and the experiment. It is observed that reducing the maximum time step improves the MAPE while simultaneously increasing the computation time.

Table 2. Comparison of Simulation Outputs with Different Input Parameter.

Number of layer	40	20	60	80	20	40	60	40	40
Max. time-step [s]	373	747	249	186	373	186	124	747	93
MAPE [%]	5.85	6.44	6.5	7.3	6.1	5.4	5.9	7.1	5.2
Computing time [s]	12.4	5.9	29.0	37.3	11.4	33.5	36.8	6.9	67.1
Simulated time up to melting last PCM [h]	8.09	6.02	8.44	8.40	5.53	8.15	8.47	8.09	8.15

As previously described, the layer height for this simulation must be chosen based on the PCM geometry. Starting from the reference simulation with 40 layers, it also becomes apparent that the results deteriorate compared to the experiment, regardless of the time step. To obtain a more accurate simulation, the simplification that the PCM elements lie within a single layer should be removed, thus increasing the computational effort. Through this analysis, an optimum between accuracy and computation time can be determined.

To establish a reference to a conventional stratified storage tank, the model was compared with an experiment involving a water-filled stratified storage tank. In this experiment, measurements were recorded during the storage charging up to 6.8 h. The charging scenario remains identical to that in the PCM storage tank, intended to be charged with warm water at 70 °C at a flow rate of 300 kg/h, with no PCM capsules in the tank. The experiment was monitored using temperature sensors, although the uppermost sensor was defective and did not provide any readings.

In Figure 7, the temperature profiles at different levels of the storage tank are displayed. The illustrations indicate that the thermocline layer moves downward uniformly over time in both the experiment and the simulation. In the simulation, a thermocline zone emerges near the inlet area, while in the experiment, it likely forms slightly lower. More detailed insights would be provided by the missing measurements. Additionally, this area may experience more mixing than the model can accurately depict. The development of devices like radial diffusers, which mitigate this effect, continues to be a significant research focus [20,21]. To represent this effect more precisely, the model equations for the inlet area should be augmented with a diffusion term.

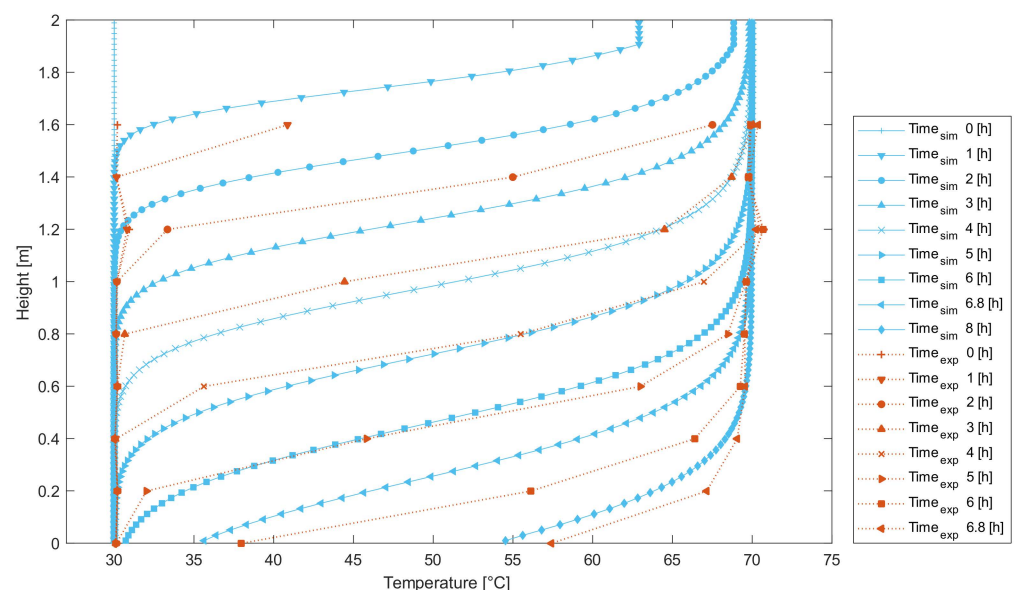


Figure 7. Temperature profiles across the height of the stratified storage tank over a period of 8 h.

Overall, the slope of the thermoclines compares very well. However, in the experiment, the thermocline zone descends slightly faster than in the simulation, leading to the exit temperature at the end of the experiment not being fully achieved in the simulation even one hour later. This temporal fluctuation of the exit temperature has also been observed in the series of experiments, where slight variations in mass flow and temperature over the duration of the experiments can become noticeable.

Despite these variations, for this experiment, the maximum absolute percentage error (MAPE) for each measurement layer at 0.2 m is a maximum of 6.2%. The mean absolute error (MAE) ranges from 0.2 °C to 5.7 °C for the measurement point in the middle of the storage tank. Despite the inaccuracies identified, the validation of the stratified storage enables us to derive insights into the behavior of pure water storage tanks versus

the behavior of those with different PCM fillings and assess their respective advantages and disadvantages.

4. Evaluating Different PCM Materials and Storage Tank Dimensions for Thermal Efficiency

Theoretically, a storage system like the one previously mentioned could be brought up to the supply temperature of a heat source. However, in practice, charging is terminated once the maximum return temperature of the source is reached. Similarly, for discharging, the storage system could theoretically be discharged down to the minimum return temperature of the consumer side, but in practice, discharging ends when the supply temperature of the consumer is undercut [29].

For a mixed-type storage tank, the return temperature increases immediately upon charging, leading to an immediate reduction in charging power. Similarly, during discharge, the discharging power quickly decreases in a mixed-type storage tank, as the supply temperature is rapidly met. Overall, this implies that mixed storage can operate only above the consumer's supply temperature and below the producer's return temperature.

Although the same limits apply to stratified storage with respect to the flow temperature of the consumer and the return temperature of the producer, these temperatures are reached much later with good stratification, and the usable heat content is significantly greater under the same conditions. Although a storage system incorporating phase change materials (PCMs) invariably enhances energy density, maintaining a large temperature difference within the storage system is also crucial. This allows for prolonged charging and discharging phases, thus enhancing the storage system's usability.

The following evaluations in Figure 8 show, for the charging process, both the cumulative energy stored in the storage tank up to that point and the temperature at the bottom of the storage tank just before reentering the heat source circuit. Compared in the figure are a pure stratified storage system (in blue) and the same storage system with 3000 PCM capsules at various melting points: 37 °C, 47 °C, 53 °C, and 60 °C. The complementary material properties can be found in Table 3. The storage system is charged under the same conditions as in a comparable validation experiment, with 70 °C at a flow rate of 300 kg/h. The simulation is terminated when the temperature at the storage system bottom reaches 60 °C. The upper plot clearly shows that the PCM increases the capacity of the storage system at the same temperature compared to the pure water storage system. The lower the PCM melting temperature, the more energy is stored within the first 3 h of charging, depending on the melting temperature of the PCM, which is reached by the heat transfer fluid, melts, and thereby absorbs significantly more energy in the melting range. Simultaneously, the lower diagram shows that just before reaching hour 4, the temperatures for the PCM-filled storage systems begin to rise, which happens about an hour later for the water storage system. This is partly because there is significantly less water in the area of the PCM packed bed, which heats up much faster despite heat transfer to the PCM in the sensible range. As soon as the melting temperature of the respective PCM is reached, the temperature at the exit stagnates at this level. The water storage system heats up continuously until it is fully charged, storing just under 100 kWh of thermal energy after 8.5 h. The PCM storage systems reach full charging incrementally with melting temperatures of 37 °C after 9.7 h with about 120 kWh, 47 °C after 11.8 h with 120 kWh, 54 °C after just under 14 h, and 60 °C after 16 h. Due to the small temperature difference between the inlet and outlet, the charging power naturally decreases, prolonging complete charging. Because of the nearly identical latent heat of fusion and specific heat capacity in the sensible ranges of the phase change materials, the total capacity is almost identical at 120 kWh.

Depending on the return temperature of the heat source, a filling with PCM at a low melting point can maintain high charging power for a longer period due to the prolonged temperature difference between the inlet and outlet into the tank, thus utilizing the higher energy density of the PCM storage system. However, choosing a PCM melting temperature

that is too high (relative to the temperatures of the heat source) can also lead to a quicker decrease in charging power in the storage system, thereby prolonging the charging process.

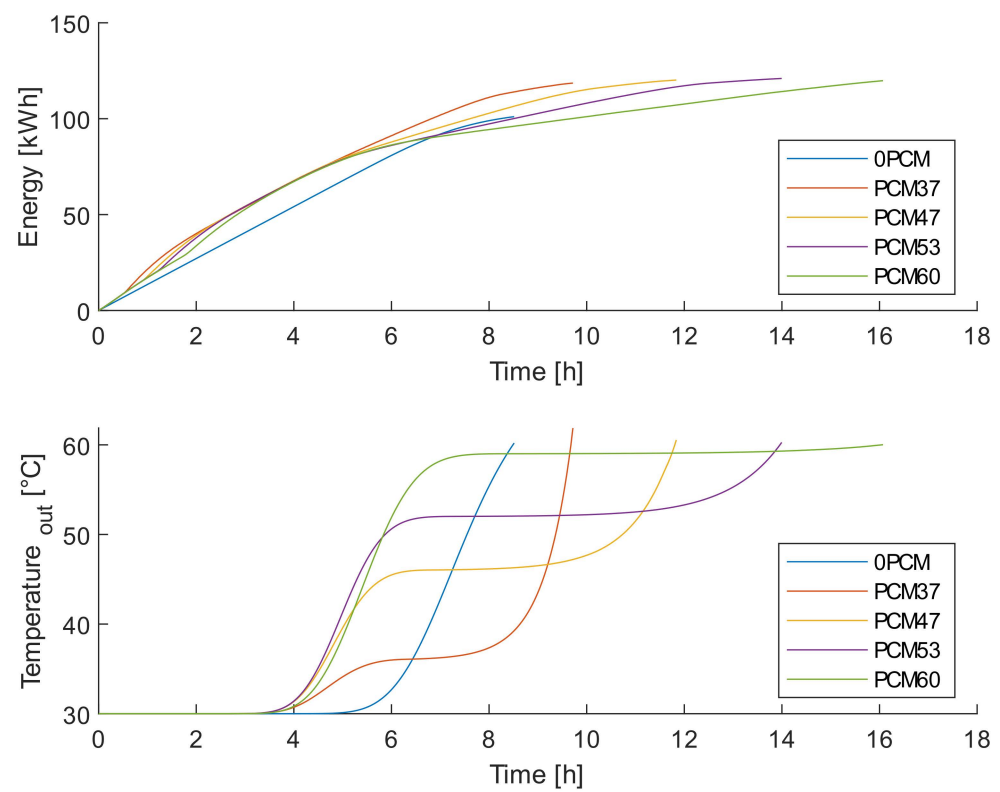


Figure 8. Accumulated energy stored in the tank and the temperature at the bottom of the tank for 3000 PCM capsules with melting points of 37 °C, 47 °C, 53 °C, and 60 °C.

Table 3. Material Properties of Crodatherm37 and Crodatherm53.

Material Property	Crodatherm37	Crodatherm53
density [kg/m ³]	957 (solid)/819 (liquid)	904 (solid)/829 (liquid)
specific heat capacity [J/kgK]	2300(solid)/1400 (liquid)	1900 (solid)/2200 (liquid)
thermal conductivity [W/mK]	0.24 (solid)/0.17 (liquid)	0.28 (solid)/0.16 (liquid)
melting temperature [°C]	37 (solid)/53 (liquid)	53 (solid)/51 (liquid)
latent heat [kJ/kg]	216–217	220–219

Figure 9 displays the variance in the number of PCMs at the same melting point of 37 °C compared to a stratified storage system. The upper plot shows that the total capacity of the storage system increases with the number of PCMs. The pure water storage system maintains the temperature at the initial level for the longest period, but the storage system with 3000 PCM capsules holds the temperature in the range of the selected melting point for the longest time. The end of charging is staggered by the number of PCMs: 6.6 h for 1000 capsules, 7.6 h for 2000 capsules, and 8.8 h for 3000 capsules. For pure water, full charging based on the criterion of 60 °C at the exit occurs after 8.5 h. However, comparing the amount of energy stored at an earlier point in time, it is evident that for the storage system with 1000 PCM capsules, nearly 95 kWh or 89% of the storage system's maximum capacity is reached by hour 4. For 2000 capsules, the same amount of energy is only reached after 5.1 h, and for 3000 capsules, after 6.2 h of charging. The maximum heat flux can be achieved at the beginning of the melting of the PCM capsules, after which it decreases as the outlet temperature rises.

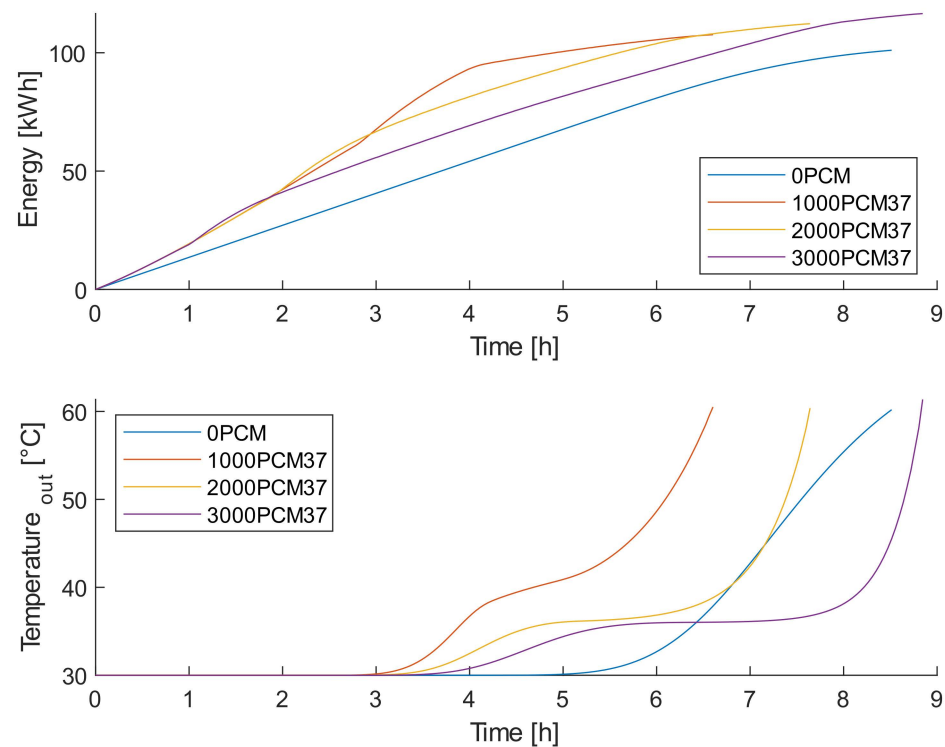


Figure 9. Accumulated energy stored in the tank and the temperature at the bottom of the tank for 1000 PCM capsules, 2000 PCM capsules, and 3000 PCM capsules with a melting point of 37 °C.

Similarly, it becomes apparent that contingent upon the characteristics of the heat source, the integration of PCM capsules can enhance the operational efficiency specific to the application. Utilizing a substantial quantity of PCM capsules augments the energy density and sustains the storage system at the melting temperature for an extended duration in the lower section of the tank. On the contrary, incorporating a minimal number of PCM capsules allows for the extraction of maximum charging capacity during the initial hours of charging, given the predefined operational conditions.

In Figure 10, two thermal storage systems with different tank geometries are compared. The charging scenario again involves a mass flow rate of 300 kg/h with water at 70 °C. One storage tank is fully filled with water and has a height of 2 m for a given diameter. The maximum storage capacity upon reaching 60 °C is approximately 98 kWh. The other thermal storage tank also has a storage capacity of 98 kWh. This one is filled with 3500 PCM capsules and, with a diameter of 1.2 m, has a height of only 1.65 m. Assuming that there are no flow-induced mixings in the PCM storage tank due to the reduced height, it becomes clear that the storage system has a charging performance very similar to that of a water tank with the same capacity. The PCM storage system begins to warm up before hour 4, but then maintains its temperature at the bottom of the tank at the melting point until the temperature rises above 37 °C after the seventh hour of charging, almost an hour later than the water storage system. The complete charging to the cutoff criterion of 60 °C is reached by the water storage system after 8 h, about 20 min before the PCM storage system.

The simulation method currently allows for filling up to three different PCM layers into any tank. The number of PCM capsules and their melting points can be varied. Figure 10 displays a water storage system and another storage system of the same size filled with PCM capsules. The lowest PCM layer contains 1500 capsules with a melting point of 37 °C, above which are 1000 capsules with a melting point of 53 °C. The top layer contains 1000 capsules with a melting point of 60 °C. The capsule packing reaches 75% of the storage tank height and is topped with water. For clarity, the illustration in Figure 11 for the PCM storage system visually represents the PCM temperature in a central block. The water and PCM zones naturally interpenetrate. The individual images show the water storage system

(top) and PCM storage system (bottom) after 1, 3, 5, and 7 h of charging under the same conditions as throughout the chapter. Independent of further analysis, the results clearly demonstrate that, with different PCM layers, a temperature stratification can be enforced around the melting points, which can be maintained for longer than in water alone. This could be beneficial for some producers or consumers in a heating system [29]. It is also evident that the thermocline zone in the PCM is substantially broader. The simulations have shown that the temperature distribution in a tank can be significantly influenced by the PCM melting temperature and the quantity of the PCM.

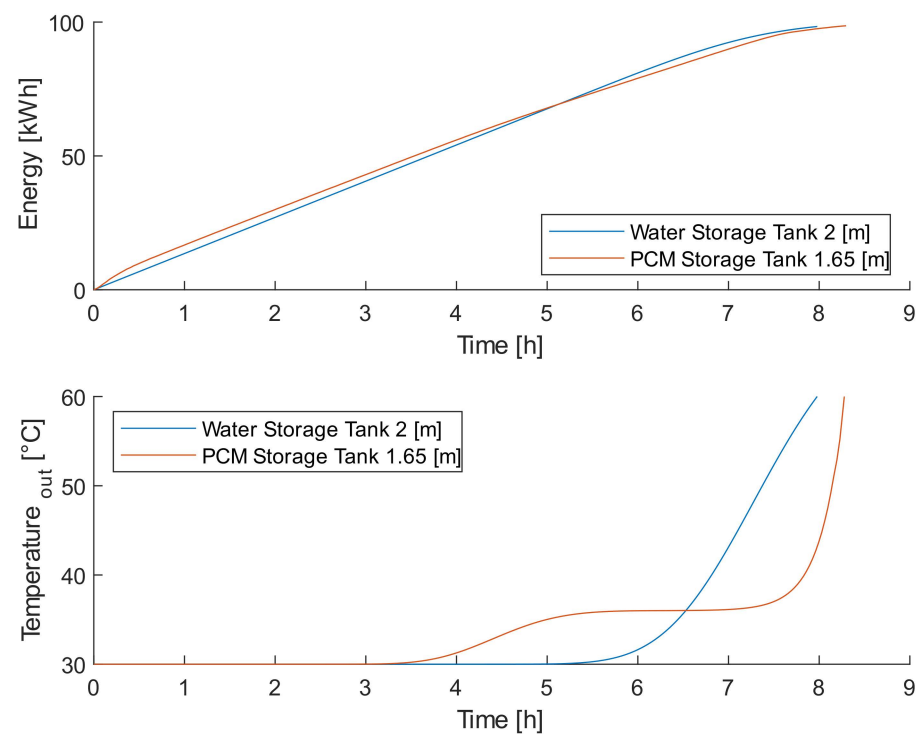


Figure 10. Accumulated energy stored in tanks with the same diameter and energy capacity, as well as the temperature at the bottom of a water storage tank with a height of 2 m and a PCM storage tank with a height of 1.65 m filled with 3500 capsules with a melting point of 37 °C.

Some limitations apply to the one-dimensional multizone model. In the water zone, only the energy equation is modeled, and no momentum equation is applied. Therefore, a uniform flow through the tank is assumed. For the water zone in the model, the one-dimensional approach is justified due to its good thermal conductivity and fluidity. However, a specific flow distribution depending on the different geometries of the inflow cannot currently be ensured. As mentioned before, when dividing the tank into any number of layers in the current model, consideration must be given to the capsule dimensions and their positioning in the tank. The capsules should lie within a single layer in the model. If a PCM capsule lies across one or more layers, no energy is exchanged within the capsule across the boundaries of those layers.

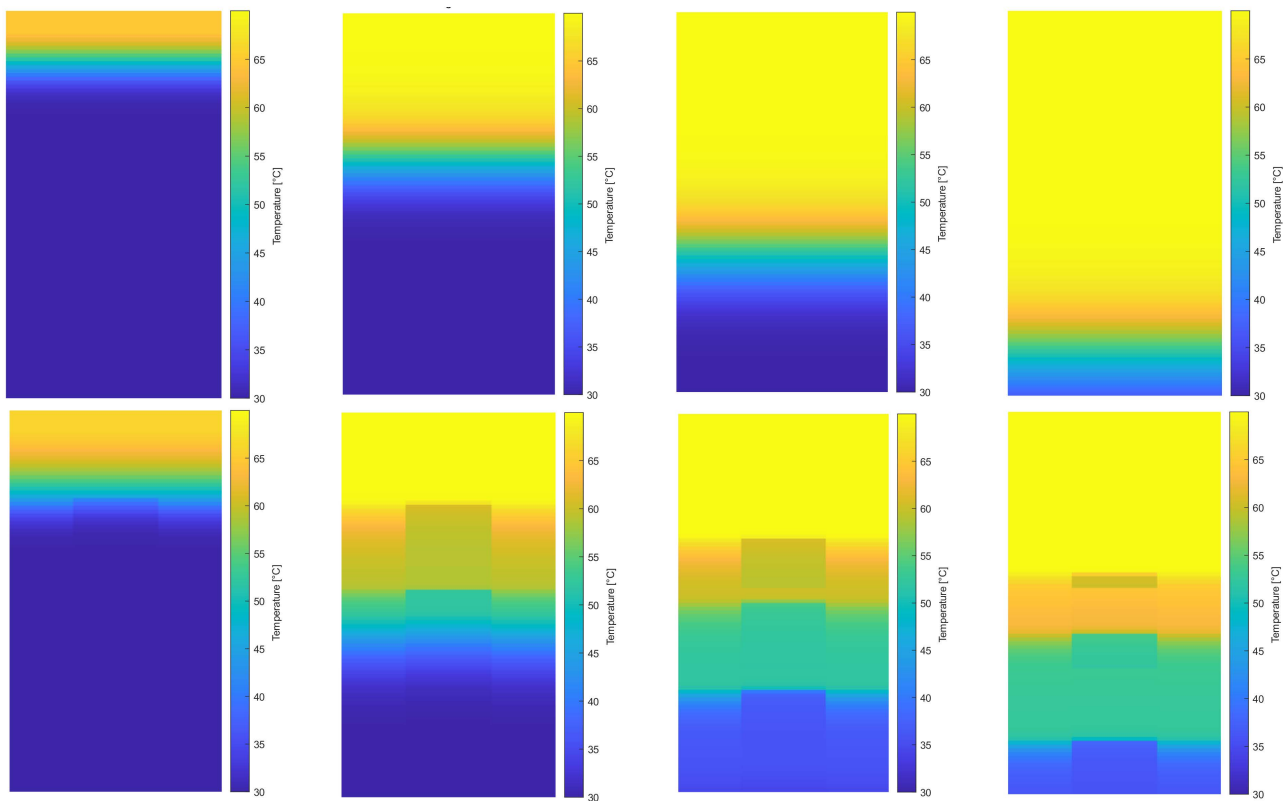


Figure 11. Comparison of temperature stratification in a water storage system (**top**) and PCM storage system (**bottom**) with different PCM layers after 1, 3, 5, and 7 h of charging under identical conditions.

5. Conclusions

The modeling described in the text offers detailed insight into the complex dynamics of energy storage systems that use PCMs. A key aspect of the model is the one-dimensional, two-zone discretization of the energy balances, which allows for a precise analysis of the temperature distribution in the water and PCMs within the storage tank.

One advantage of the model is its ability to represent extensive scenarios based on a manageable number of input conditions, while maintaining the flexibility to adapt to different tank geometries and varying numbers of PCM capsules. This flexibility enables the system to be optimized for different applications and operating conditions, which is particularly important, as no energy storage system is universal. The ability to model capsules with different melting points in specific layers of the storage system provides additional options for optimizing energy storage and release.

A critical point in modeling such PCM systems is to accurately represent the energy transfer between water and PCM capsules. The model simplifies various heat transfer mechanisms based on previous studies by representing the transfer from the capsule shell to the inside with just one coefficient, which depends on the capsule shape and the thermal conductivity of the PCM material.

Experimental validation is essential to verify the model assumptions and to confirm the accuracy of the simulation results. The model was validated with experimentally measured data, and the deviations were below 6%. Using the model, the study shows that layering in the storage tank can be achieved through a filling with different PCM melting points without compromising the maximum storage capacity. For example, the temperature at the tank outlet can be maintained at the melting point temperature of the PCM for up to 20% longer while storing up to 14% more energy at this point. The implementation of the model into a larger heating system network, and, if necessary, the expansion to a multidimensional model, which is relevant for thermal storage systems with stratification lances, could be made. The optimization of PCM configurations specially customized to

consumers and producers can be examined, demonstrating system-relevant improvements and revealing application-related enhancements over an extended period. By gaining more detailed insights into PCM storage technology and optimizing it for efficiency, energy losses can be reduced, and the use of renewable energies that rely on storage technology can be improved. Our model makes it possible to examine flexible adjustments to tank geometry and PCM configuration more precisely and, in a further step, customize them to specific heat generation systems and consumer needs, such as solar heat combined with a heat pump and surface heating. This not only improves the efficiency of the storage tank itself, but also enhances the efficiency of individual producers and consumers, who can benefit from a PCM-defined temperature profile in the storage tank. In addition, economic and ecological aspects, such as operating costs and the reduction of CO₂ emissions, should also be improved. Our research provides an innovative foundation and enhances the integration of renewable energies.

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Nomenclature

Symbol	Unit	Quantity
a	m ² /s	thermal diffusivity
A	m ²	area
c_p	J/(kg K)	specific heat capacity at constant pressure
d	m	diameter
d_k	m	diameter of equivalent geometric surface
E	J	energy
F_{form}	-	form factor
g	m/s ²	gravitational acceleration
h	m	height
h	J/m ³	sensible volumetric enthalpy
l	m	length
m	kg	mass
$\dot{m}$	kg/s	mass flow
Q	J	heat
$\dot{Q}$	J/s	heat flux
R	K/W	thermal resistance
r	m	radius
T	K	temperature
t	s	time
U	W/(m ² K)	overall heat transfer coefficient
u	m/s	velocity magnitude
V	m ³	volume
α	W/(m ² K)	heat transfer coefficient
ε	-	porosity
λ	W/(m K)	thermal conductivity
μ	kg/(m s)	dynamic viscosity
ν	m ² /s	kinematic viscosity
ρ	kg/m ³	density
ax	axial	

<i>amb</i>	ambience
<i>C</i>	capsule
<i>ch</i>	charge
<i>down</i>	downwards
<i>dis</i>	discharge
<i>eff</i>	effective
<i>ext</i>	extern
<i>exp</i>	experiment
<i>Fl</i>	fluid
<i>exp</i>	experiment
<i>+g</i>	with gravity
<i>i</i>	number of layer
<i>in</i>	intern
<i>l</i>	liquid
<i>lam</i>	laminar
<i>m</i>	melting
<i>n</i>	numbers of layer
<i>PCM</i>	phase change material
<i>s</i>	solid
<i>sim</i>	simulation
<i>Tank</i>	tank
<i>up</i>	upwards
<i>turb</i>	turbulent
<i>W</i>	wall
<i>zero-g</i>	without gravity

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