

Article

Performance Evaluation of a Packed Bed Latent Thermal Storage System Using Superellipsoidal PCM Capsules

Matti Grabo ^{1,*}, Lennart Kuckuck ² and Eugeny Y. Kenig ² 

¹ Competence Center for Sustainable Energy Technology, Paderborn University, Warburger Straße 100, 33098 Paderborn, Germany

² Chair of Fluid Process Engineering, Faculty of Mechanical Engineering, Paderborn University, Warburger Straße 100, 33098 Paderborn, Germany; eugen.y.kenig@upb.de (E.Y.K.)

* Correspondence: matti.grabo@upb.de

Abstract

Two crucial yet opposing design criteria govern the performance of packed bed latent thermal energy storage systems (PBLTESS): energy storage capacity and thermal power. While the former depends on the packing density of the phase change material (PCM) capsules forming the packed bed, the latter is influenced by the surface-area-to-volume ratio (SVR) of these capsules. This study introduces novel superellipsoidal geometries for PCM capsules to address both these factors and quantifies the impact of design parameters on both mentioned performance criteria. First, by using discrete element method (DEM) simulations, we performed virtual bed filling experiments and generated packed beds from 116 superellipsoidal designs with similar volume. These simulations revealed a maximum packing density of 65.2%—significantly higher than conventional spherical capsule designs. Validation through bed filling experiments using 3D-printed superellipsoids confirmed the results of the DEM simulations, with an average deviation of less than 5%. Additionally, the SVR of each superellipsoidal design was determined through CAD analyses. Subsequently, six superellipsoidal designs as well as a spherical design were selected for further investigation using a 1D PBLTESS model to simulate charging and discharging. With up to 85% higher storage capacity (due to increased packing density) and up to 50% higher thermal power (resulting from enhanced heat transfer), the superellipsoidal geometries clearly outperformed the spherical design.

Keywords: thermal storage; latent heat; phase change materials (PCM); heat transfer; packed beds; superellipsoids; discrete element method



Academic Editor: Chi-Ming Lai

Received: 5 May 2026

Revised: 2 June 2026

Accepted: 22 June 2026

Published: 2 July 2026

Copyright: © 2026 by the authors.

Licensee MDPI, Basel, Switzerland.

This article is an open access article distributed under the terms and conditions of the [Creative Commons Attribution \(CC BY\)](https://creativecommons.org/licenses/by/4.0/) license.

1. Introduction

With a share of only 14% of renewable energy sources in the heat production mix, thermal energy consumption contributed 37% to the overall global CO₂ emissions in 2024 [1]. One reason for the limited use of renewable energy for heating and cooling is its volatility, which can lead to an imbalance between supply and demand. Therefore, efficient storage solutions are needed to ensure that demand is always met, even when fluctuating energy sources are temporarily unavailable.

Thermal storage technologies are generally subdivided into sensible, latent, and chemical storage concepts. While sensible storage systems are commonly used and low-cost, their storage capacity is limited to the specific sensible heat capacity of the storage material [2]. Chemical storage systems offer a much higher storage capacity; however, they are still at

a relatively low technological maturity level and, therefore, quite expensive [3]. Latent thermal energy storage systems (LTESS) range between both aforementioned technologies and represent a good compromise between capacity and cost. LTESS utilize the latent energy of solid–liquid phase changes and provide significantly higher storage capacity than sensible thermal energy storage systems [4].

Different configurations of LTESS exist. One example is the shell-and-tube design, which resembles a conventional shell-and-tube heat exchanger, except that the shell side contains a phase change material (PCM) instead of another heat transfer fluid (HTF). Another concept for LTESS is direct-contact storage, in which the HTF is in immediate contact with the PCM. In this work, we focus on another common design, the packed bed latent thermal energy storage system (PBLTESS), which consists of a tank containing an HTF and encapsulated PCM capsules arranged as a packed bed. A schematic of a PBLTESS is shown in Figure 1.

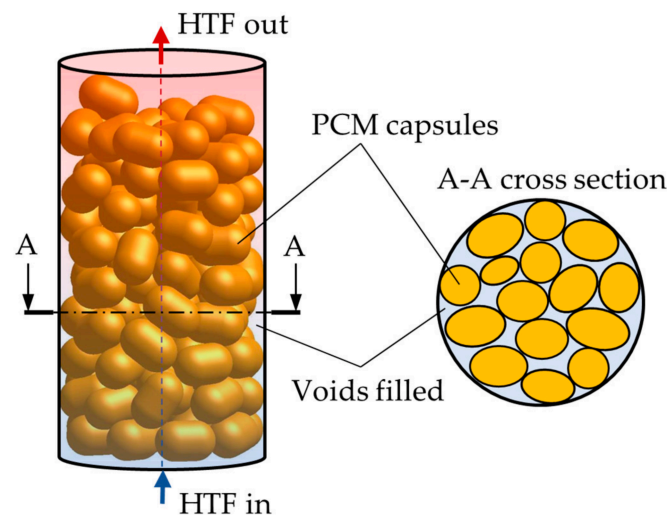


Figure 1. Schematic of a packed bed consisting of PCM-filled capsules.

Most studies on PBLTESS, both experimental and numerical, employ spherical PCM capsules. For example, a review on LTESS based on PCM-filled capsules by Regin et al. [5] includes only two out of 18 surveyed studies that consider capsules of non-spherical geometry. Similarly, a review on the modeling of PBLTESS by de Gracia and Cabeza [6] only mentions models for spherical capsules. Mawire et al. [7] experimentally investigated different setups of PBLTESS by varying the HTF flow rates and the PCM; however, they also studied only spherical capsules. Alptekin and Ezan [8] evaluated the energetic and exergetic performance of a PBLTESS combined with a solar thermal collector under varying flow rates and for different capsule sizes. They found that higher flow rates and smaller capsule diameters had a positive effect on the performance of their investigated system. Again, spherical capsules were studied. Suresh and Saini [9] investigated a combined sensible-latent heat storage concept as part of a solar thermal collector system. They studied the influence of different PCM volume fractions on the system performance and varied the mass flow rate of the HTF. Only spherical capsules were used here as well. Further studies in which spherical PCM capsules were employed are described in Refs. [10–14].

Although the design of the spherical PCM capsule appears attractive due to its simplicity, it is actually the least suitable geometric shape that could be used for PBLTESS. The reason for this claim becomes clear by taking a closer look at the performance criteria of LTESS: they should achieve a high volumetric energy storage capacity while also providing high thermal power during charging and discharging [15]. Along with the capsule volume and shape, the storage capacity depends on the number of capsules per volume inside

the storage tank and therefore depends on the packing density, which varies for different geometrical bodies. The thermal power, on the other hand, is governed by operational parameters such as mass flow rate and temperature difference, but also by the heat transfer area between the packed bed and the HTF, which in turn depends on the geometrical shape of the packed elements. The geometry of the PCM capsules thus influences both storage capacity and thermal power and hence represents a crucial design parameter for PBLTESS [16].

While random packings of spheres can achieve relatively high packing densities of up to 64% [17], they also have a great disadvantage: their surface-area-to-volume ratio (SVR) is the lowest among all geometrical bodies. This not only has a negative effect on the heat transfer rate at the capsule surface but also results in high internal thermal resistance due to the substantial distance between the capsule surface and its center. A non-spherical body with a similar volume as a sphere will always be “thinner” in the sense that the minimum distance from its center to its surface is shorter than that of a sphere (i.e., the sphere radius). Since the net thermal resistance is determined by the thickness of the conducting material, PCM spheres inherently need a longer time to completely change their state than other capsule geometries. Therefore, using PCM capsules that deviate from the spherical shape gives a clear advantage in thermal power. The goal of our study was to identify capsule designs that achieve packing densities similar to or greater than those of spheres while offering higher thermal power.

Few authors investigated alternative capsule designs. Awasthi et al. [18] numerically studied different cylindrical PCM capsules with sinusoidal lateral surfaces. They found that the amplitude of the sinusoidal surfaces significantly affects the melting duration, while the number of sinusoids has only a small impact.

Inspired by the principles of bionics, Cheng and Zhai [19] proposed a design based on a red blood cell. They compared the heat transfer and phase change durations of a blood-cell-shaped capsule with other geometries, such as torus, sphere, and cylinder, and found that the blood cell shape exhibited the best thermal performance, while the spherical and cylindrical capsules performed rather poorly. However, their experimental and numerical studies were conducted only on individual capsules, whereas the performance in a packed bed configuration was not evaluated.

Heinz and Moser [20] conducted both experimental and simulative investigations using a commercially available, non-spherical PCM capsules, the HeatSel® by Axiotherm GmbH [21]. The focus of their work was on developing a numerical model, which they planned to use in full-system simulations of cooling applications. They were able to achieve good accuracy (less than 1 K deviation) after performing some parameter fitting, which was necessary due to the modeling assumption of spherical capsules. Although the validation was successful, they did not investigate other possible capsule geometries.

In an attempt to improve thermal performance, Jia et al. [22] investigated the effect of dimples on spherical capsules based on large eddy simulations. They found that dimples increase heat transfer by up to 28% and reduce the complete phase change duration by about 19%. However, the simulations were performed only on individual capsules, and the effect of dimpled spheres in packed beds was not investigated.

Sponagle et al. [23] developed a complementary modeling approach for PBLTESS, utilizing 2D finite element simulations for the heat transfer processes inside the investigated cylindrical PCM capsules and 1D finite volume simulations for the HTF. They were able to validate their model with good accuracy while simultaneously reducing the computational effort, enabling the model to be used for optimization or control applications.

Even though the studies mentioned above investigate non-spherical PCM capsules for PBLTESS, their focus was not on a systematic investigation of the effect of capsule

shape on the performance of PBLTESS. In order to close this gap and to identify promising capsule designs that enhance the performance of PBLTESS, 116 different geometries based on so-called superellipsoids were systematically investigated in this study. Superellipsoids are a group of geometrical objects defined by a fixed set of five design parameters and offering a wide variety of different shapes. All considered geometries had the same volume. The goal was to evaluate each geometry with respect to its SVR and packing density. To achieve this, the geometries were first generated as an STL file using MATLAB R2021b and then exported into a CAD format using Autodesk Inventor Professional 2024. Based on the CAD model, the surface area required to calculate the SVR could be determined. Next, the superellipsoidal CAD models were imported into Simcenter STAR-CCM+ 2020.2 and used to perform virtual bed filling experiments applying a discrete element method (DEM) in order to determine the achievable packing density of each of the 116 individual geometries. The DEM simulations were validated against measured data retrieved from a scaled-down experimental setup with high accuracy. Finally, six novel capsule designs were numerically studied and compared to spherical capsules using a transient thermal model for PBLTESS developed by Grabo et al. [24]. The novelty of this work lies in the systematic evaluation of various superellipsoids with regard to their thermal performance in PBLTESS.

2. Methods

2.1. Superellipsoids

To identify PCM capsule geometries that can achieve both high thermal power and energy density, novel designs based on superellipsoids were examined in a parametric study. Superellipsoids are geometrical bodies that are defined by three parametric equations as follows:

$$\begin{aligned} x(v, w) &= a \cdot \operatorname{sgn}(\cos(w)) \cdot |\cos(w)|^n \cdot \operatorname{sgn}(\cos(v)) \cdot |\cos(v)|^e \\ y(v, w) &= b \cdot \operatorname{sgn}(\cos(w)) \cdot |\cos(w)|^n \cdot \operatorname{sgn}(\sin(v)) \cdot |\sin(v)|^e \\ z(v, w) &= c \cdot \operatorname{sgn}(\sin(w)) \cdot |\sin(w)|^n \end{aligned} \quad (1)$$

for $-\pi \leq v < \pi$ & $-\pi/2 \leq w \leq \pi/2$

These equations depend on only five design parameters, yet they allow for the creation of a wide variety of different geometries. Here, a , b , and c represent the maximum length of the superellipsoid geometry in each spatial direction, while e and n are so-called shape factors that determine the roundness of the resulting body. The function arguments v and w represent surface grid parameters. An example of a superellipsoid along with its defining parameters as well as some other geometries that can be generated by using Equation (1) are shown in Figure 2.

The volume of superellipsoids V_S can be determined by:

$$V_S = \frac{2}{3}abcnB\left(\frac{e}{2}, \frac{e}{2}\right)B\left(n, \frac{n}{2}\right) \quad (2)$$

where B is the beta function (see details in, e.g., Ref. [25]).

Two aspect ratios were defined in order to reduce the number of parameters studied:

$$\beta = \frac{a}{b} \quad (3)$$

$$\gamma = \frac{a}{c} \quad (4)$$

By rearranging Equation (2) for a , the superellipsoid can be described by its volume, two aspect ratios and two shape factors. This allows superellipsoids to be generated

without having to explicitly define the lengths of their axes, and it enables an effortless size scaling by specifying the volume.

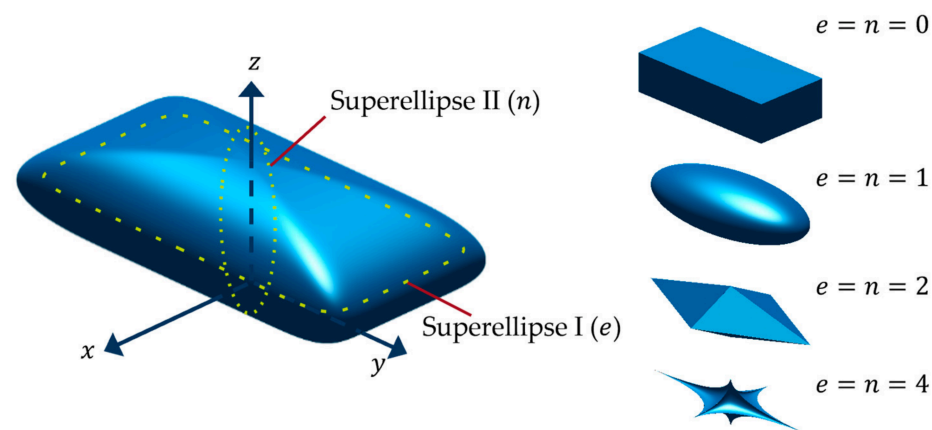


Figure 2. Superellipsoid with its two defining superelliptic curves with parameters $a = 2$, $b = 4$, $c = 1$, $e = 0.2$ and $n = 1$ (left) as well as other possible superellipsoidal geometries showing the influence of the shape parameters (right).

2.2. Evaluation Criteria

Two parameters influencing the performance of the overall PBLTESS which are inherently based on the geometry of the PCM capsules are the volumetric energy density (i.e., the storage capacity per unit of volume) and the thermal power. The former depends on the packing density, which is defined as the ratio of the overall volume of the packed elements (i.e., the overall number of PCM capsules N_C multiplied by the volume of one capsule V_C) and the overall packed bed volume V_{PB} :

$$\varepsilon = \frac{N_C V_C}{V_{PB}} = \frac{N_C V_C}{H_{PB} A_{PB}} \quad (5)$$

where H_{PB} and A_{PB} are the height and the cross-sectional area of the packed bed.

The geometrical influence on thermal performance stems from the heat transfer rate $\dot{Q}$ between the packed bed and the HTF at the surface of the capsules:

$$\dot{Q} = Ah\Delta T \quad (6)$$

where A is the heat transfer area, h is the heat transfer coefficient, and ΔT is the temperature difference between the bed and the HTF. Both the surface area and the heat transfer coefficient depend directly on the capsule geometry. An integral description of this geometry is given by the SVR, which is defined as:

$$SVR = \frac{A_C}{V_C} \quad (7)$$

where A_C is the surface area of one individual capsule. In this work, we used the SVR to evaluate the surface geometry influence on the heat transfer and thus the thermal power.

The SVR could easily be derived from the CAD models of the considered capsule geometries. In order to determine the packing density for each individual capsule design, DEM simulations were performed, which are described in the following section.

2.3. Generation of Packed Beds with DEM

The packed bed density is unique for each superellipsoid and cannot be determined without either experiments or simulations. In this work, virtual filling experiments were

performed with all 116 considered superellipsoids using a DEM that is available in the commercial simulation software STAR-CCM+.

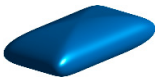
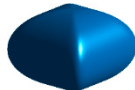
First, Equation (1) was implemented in MATLAB as an executable script that creates the surface meshes of the superellipsoids. These meshes were then exported to an STL format, which is a common standard for CAD data exchange. The STL-files were subsequently imported into STAR-CCM+ to perform DEM simulations, through which the packing densities of different superellipsoids were determined. The DEM approach used in this work is based on the method proposed by Feng et al. [26], which was specifically developed for convex geometries and is already implemented in STAR-CCM+. The acting forces considered in the model were the contact forces for element-to-element and element-to-wall collisions as well as gravitation. The contact forces were accounted for using the linear spring-contact model, a variation in the spring-dashpot model (see Ref. [27]). The DEM simulations were based on the properties of polyamide 12, the material used in the validation study described below. These properties are listed in Table 1.

Table 1. Properties of discrete elements used in DEM simulations.

Property	Value
Density	1040 kg/m ³
Young's modulus	4.63 GPa
Yield strength	44.4 MPa
Poisson's ratio	0.393
Coefficient of friction	0.312
Normal spring constant	10 kN/m
Tangential spring constant	8 kN/m
Coefficient of restitution	0.65

Before performing the DEM simulations with all 116 superellipsoidal geometries, the DEM approach was validated through simple bed filling experiments. In these experiments, small superellipsoidal pellets made of polyamide 12 and produced via 3D printing were used. Each geometry considered for the validation procedure had the same volume of approximately 7.7 mL, which is based on a 1:5 scale-down of a commercial PCM capsule containing approximately 1 kg of PCM. The parameters of the superellipsoid geometries considered for the validation of the DEM simulations are shown in Table 2.

Table 2. Superellipsoids used in the DEM validation study.

Geometry	Parameters				Geometry	Parameters			
	β	γ	e	n		β	γ	e	n
1 	2	3	0.2	1	4 	1	1	0.2	1
2 	2	0.4	0.2	1	5 	2	3	0.2	1.667
3 	6	2	0.2	1	6 	6	2	0.2	1.667

For each of the geometries listed in Table 2, 350 pellets were produced using 3D printing and subsequently used for filling tests in the experimental setup shown in Figure 3, left. First, the pellets were filled into the pellet container. Then the cover was removed so that the pellets fell into the lower container, which had a diameter of 16 cm. Once the pellets had settled into a packed bed, the resulting height of the bed was measured. This process was performed five times for each individual geometry, yielding an average bed height calculated from the measured values. The resulting average was then used to determine the packing density of each superellipsoid using Equation (5).

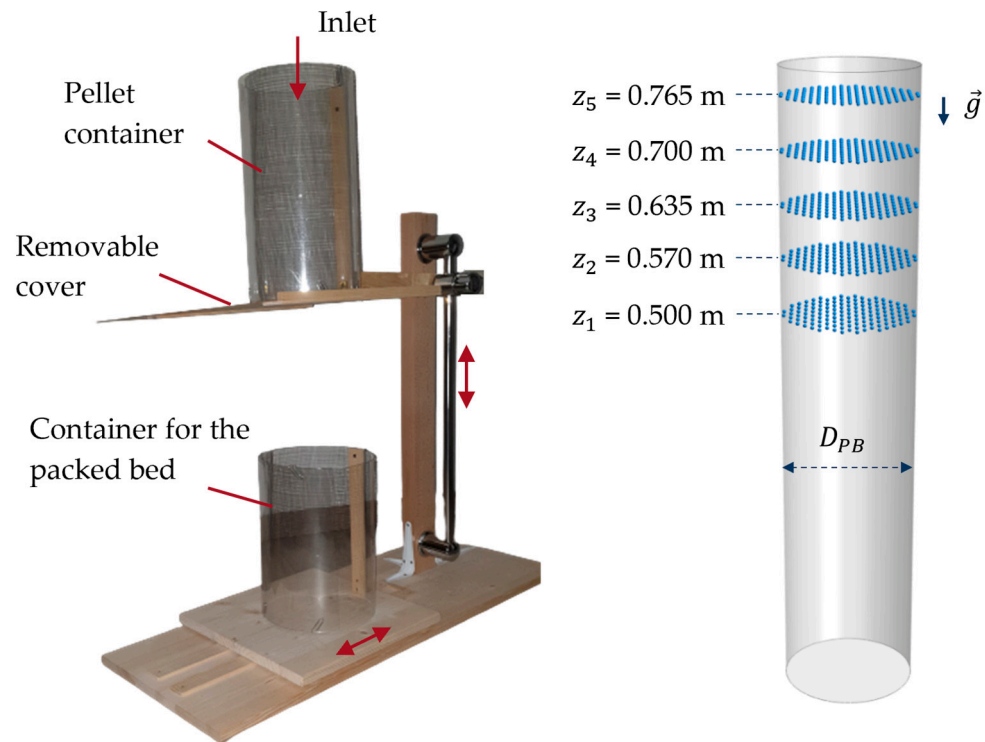


Figure 3. Setup for bed filling experiments (left), as well as tank geometry and injector locations used in the DEM simulations (right).

In the subsequent DEM simulations, the containers for the pellets and the packed bed were modeled as one single cylinder, with injection points defined at five different heights in its upper half, as shown in Figure 3, right. A total of 350 individual pellets were randomly distributed across 685 injectors over a period of four seconds. They fell downward due to gravity, where they formed a packed bed. The number of elements was chosen so that the ratio of packed bed height to axial length of a single pellet was at least 5 or greater.

The experimental and DEM simulation results are shown in Figure 4. It can be seen that the measured and simulated packing densities show good qualitative agreement. The average deviation between the simulations and the filling experiments was 4.8%, indicating successful validation of the chosen DEM approach.

2.4. Parametric Study

The validated DEM approach was subsequently applied in a parametric study to investigate how the geometrical parameters β , γ , e and n influence the bed packing densities of various superellipsoids. In this study, the aspect ratios β and γ were varied between 0.4 and 8.0, while the shape factor n was varied between 1.0 and 1.667. The second shape factor e was kept at a constant value of 0.2. This selection of values was based on a preliminary analysis of packed beds filled with superellipsoids, which showed that values of e and n

close to 0 or 2 result in voluminous, cubic geometries with large flat surfaces, as shown in Figure 2, right. Such shapes impede fluid flow in packed beds. Furthermore, if the shape parameters exceed 2, the resulting superellipsoids take a star-shaped form, which can lead to mechanical instability and manufacturing issues and is therefore not suitable for PCM capsules.

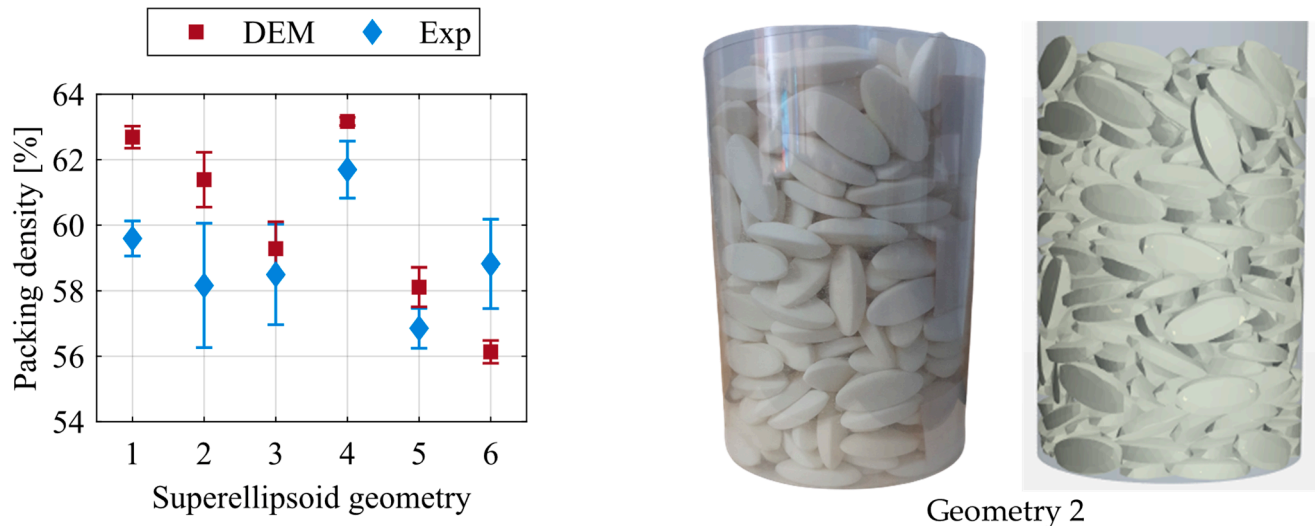


Figure 4. DEM and experimental results for the geometries given in Table 2 (left) and a packed bed created by experiment and by DEM (right).

The choice to keep one of the shape factors at a constant value was based on studies by Delaney and Cleary [28] and Zhao et al. [29], who investigated packed beds consisting of superellipsoids. Although they found that low values for both shape factors lead to slightly higher packing densities, which has a positive effect on the energy density of PBLTESS, the resulting geometries are cuboid-shaped and exhibit poor heat transfer properties. To avoid such geometries while still enabling relatively high packing densities, one the shape factor e was therefore chosen as low as possible.

The values used for the geometrical properties of the investigated superellipsoids are given in Table 3. Although all possible combinations of parameters would result in a total of 192 superellipsoids, some geometries were discarded due to apparent shortcomings regarding their suitability as PCM capsules (i.e., superellipsoids with axis lengths over 30 cm, which was a constraint stemming from the manufacturing process). The volume of all superellipsoids considered corresponded to that of the validation study.

Table 3. Aspect ratios and shape factors considered in the parametric study.

Parameter	Values							
Aspect ratio β	0.4	0.7	1.0	2.0	3.0	4.0	6.0	8.0
Aspect ratio γ	0.4	0.7	1.0	2.0	3.0	4.0	6.0	8.0
Shape factor e	0.2							
Shape factor n	1.0	1.25	1.667					

A total of 116 different superellipsoid geometries (46 for $n = 1$, 39 for $n = 1.25$ and 31 for $n = 1.667$) were considered, and the respective packing density resulting from the DEM filling simulations performed with each of these geometries was evaluated. Additionally, the SVR was determined for all geometries based on their CAD models.

2.5. Thermal Model of PBLTESS

Charging and discharging simulations were performed for each geometry using the SVR and the packing densities determined through the DEM analysis. The thermal simulations were performed using an extended version of a PBLTESS model developed by Grabo et al. [24]. This model is a two-equation model and based on the concentric dispersion approach for thermal simulations of packed beds [30]. It involves solving one equation for the HTF and one for the PCM capsules. The former is given as:

$$(1 - \varepsilon)\rho_f c_{p,f} \frac{\partial T_f}{\partial t} = (1 - \varepsilon)k_f \frac{\partial^2 T_f}{\partial x^2} - \rho_f c_{p,f} u_f \frac{\partial T_f}{\partial x} + \frac{A_{PB}}{V_{PB}} h(T_{PB} - T_f) \quad (8)$$

where ρ is density, c_p is the specific heat capacity, t is time, k is thermal conductivity, x is the spatial coordinate in the direction of HTF flow, u is the HTF superficial flow velocity, while the indices f and PB indicate the HTF and the packed bed, respectively. The governing equation for the PCM capsules is given as:

$$c_{vol} \frac{\partial T_{PB}}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} (\lambda r^2 \frac{\partial T_{PB}}{\partial r}) - \rho_l L \frac{\partial g_l}{\partial t} \quad (9)$$

where c_{vol} is the volumetric heat capacity, r is the radial coordinate, λ is the mixture thermal conductivity, ρ_l is the density of the liquid PCM, L is the latent heat of fusion and g_l is the liquid fraction. The mixture quantities c_{vol} and λ are defined as follows:

$$c_{vol} = (1 - g_l)\rho_s c_{p,s} + g_l \rho_l c_{p,l} \quad (10)$$

$$\lambda = (1 - g_l)k_s + g_l k_l \quad (11)$$

where indices l and s indicate the liquid and the solid phase of the PCM, respectively.

The liquid fraction was defined as a linear function of temperature:

$$g_l = \begin{cases} 0 & \text{if } T < T_s \\ \frac{T - T_s}{T_l - T_s} & \text{if } T_s \leq T \leq T_l \\ 1 & \text{if } T > T_l \end{cases} \quad (12)$$

where T_s and T_l are the solidus and the liquids temperature, which are properties of the selected PCM.

Both governing equations are coupled via the boundary condition for Equation (9) and the source term in Equation (8):

$$k_C \frac{\partial T_{PB}}{\partial r} \bigg|_{r=R_C} = h(T_f - T_{PB}) \quad (13)$$

where k_C is the thermal conductivity of the encapsulation material and R_C is the outer radius of the PCM capsule shell.

The heat transfer coefficient h was determined using the Nusselt correlation for mixed convection according to Churchill [31]. The Nusselt number for forced convection was calculated according to Gnielinski [32,33], while for natural convection, the correlation of Kast et al. [34] was used.

When applying these model equations, the following assumptions were made:

- Perfect thermal insulation of the storage tank (no energy losses to the environment);
- No temperature gradients in radial direction;
- Negligible subcooling effects;

- Negligible natural convection effects inside PCM capsules due to the expected formation of a mushy zone;
- The PCM capsules can be approximated by spherical shells, which have the same surface area and contain the same PCM volume as the original geometry (cf. Ref. [24]);
- Homogenous porosity within the packed bed;
- The whole packed bed surface area is thermally active;
- Negligible thermal radiation;
- Thermal conduction through capsule contact points can be neglected due to low thermal conductivity and small temperature differences;
- Possible air enclosures inside the capsules are not considered; and
- Temperature-independent material properties due to small temperature differences (20 K or less).

The governing equations given above were discretized using two different finite differences schemes. The equation for the HTF (Equation (8)) was discretized using the explicit finite differences method, while the equation for the PCM capsules (Equation (9)) was discretized using the implicit finite differences method. This allowed both domains to be evaluated in a time-consistent manner, while avoiding any additional iterations between the HTF and capsule shell domain. The solution methods were implemented in MATLAB R2021a. Regarding the size of the temporal and spatial steps, a grid independence study was performed, which showed that a time step Δt of 2.5 s and spatial steps of $\Delta x = 3.72$ mm and $\Delta r = 0.156$ mm were sufficient. The numerical algorithm as well as the validation procedure, which revealed an average deviation between measured and simulated data of less than 10%, are given in detail in Ref. [24].

3. Results and Discussion

3.1. Packing Density and Surface-Area-to-Volume Ratio

The results of the DEM simulations are illustrated in Figure 5, which includes color plots of the packing densities for all considered parameter combinations. The highest packing densities can be observed for aspect ratios between 0.4 and 2, corresponding to bulkier geometries. Furthermore, when β and γ differ greatly from each other, the packing density is quite low, as is the case for, e.g., $\beta = 8$ and $\gamma = 1$. Compared to the aspect ratios, increasing the form factor does not appear to have a significant effect on the packing density, as the three graphs representing the three different values of n show quite similar trends.

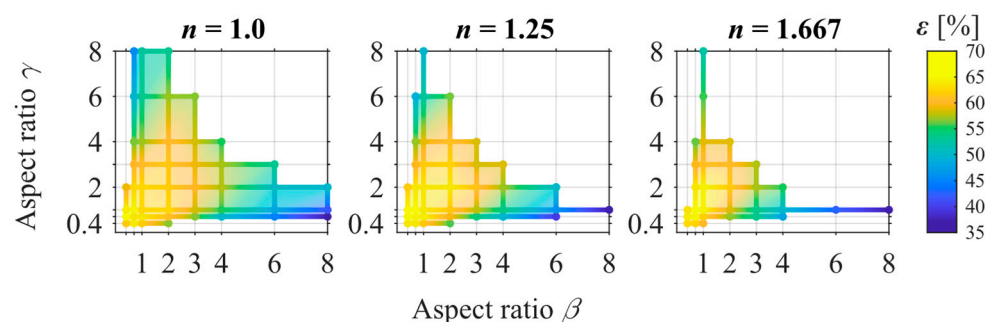


Figure 5. Impact of superellipsoid aspect ratios β and γ as well as shape factor n on the packing density ϵ (each grid point represents one superellipsoid).

To evaluate the SVR of the superellipsoids under consideration, they were scaled to correspond to the volume of a PCM capsule containing approximately 1 kg of PCM. This adjustment ensured that the absolute SVR values more accurately reflect those of real PCM capsules, as would be used in PBLTESS. Figure 6 shows the SVR results for the same superellipsoid geometries. The color plots appear to be reversed compared to Figure 5—

larger aspect ratios produce flatter and thinner geometries, which tend to have a higher SVR. Here, too, the effect of the shape factor does not appear to play any significant role.

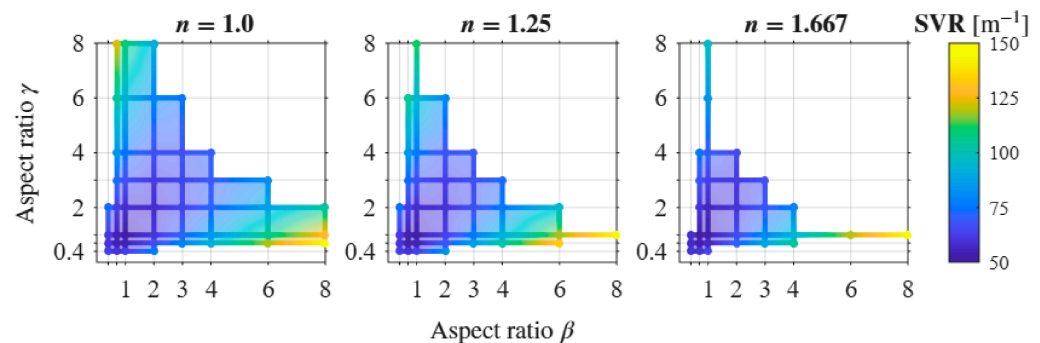


Figure 6. Impact of superellipsoid aspect ratios β and γ as well as shape factor n on the surface-area-to-volume ratio SVR.

Altogether, the highest observed packing density was 65.22% resulting from a parameter combination of $\beta = 1$, $\gamma = 0.7$, $e = 0.2$ and $n = 1.667$. The corresponding SVR value was 53.73 m^{-1} , which was significantly lower than the value for the geometry with the highest SVR of 144.0 m^{-1} , obtained from the parameter combination $\beta = 1$, $\gamma = 8$, $e = 0.2$ and $n = 1.667$. However, the latter combination achieved a packing density of only 37.23%, which is relatively low and corresponds to about half the packing density of a bed consisting of randomly packed spheres. Both geometries are displayed in Figure 7. The superellipsoid achieving the highest packing density resembles a bulky octahedron, while the one with the highest SVR is shaped like a flat octahedron.

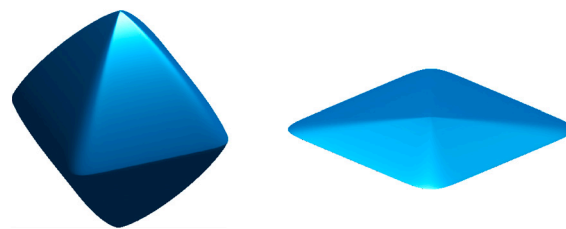


Figure 7. Superellipsoids achieving the highest packing density with $\beta = 1$, $\gamma = 0.7$, $e = 0.2$ and $n = 1.667$ (left) and the highest SVR with $\beta = 1$, $\gamma = 8$, $e = 0.2$ and $n = 1.667$ (right).

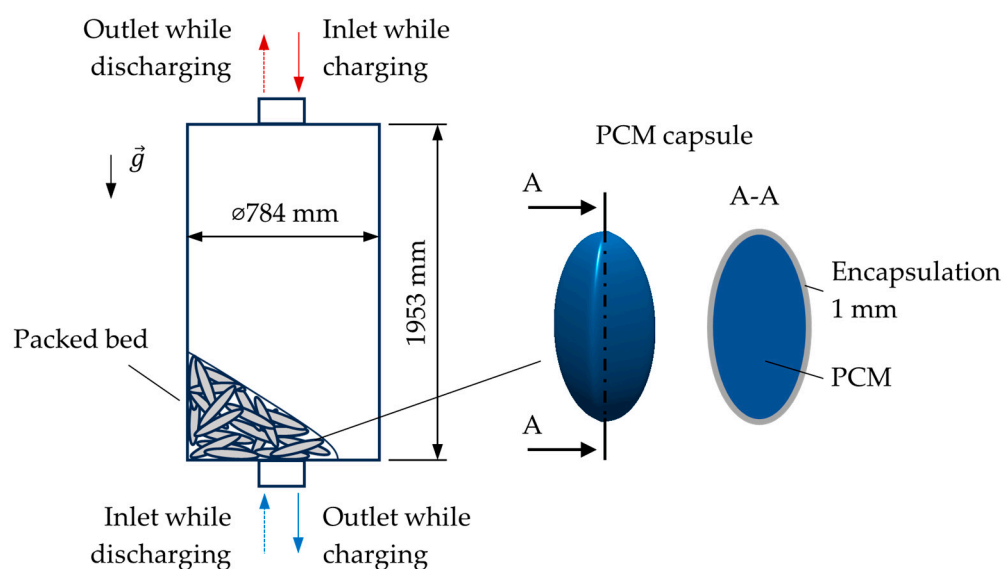
3.2. Thermal Performance of Selected Superellipsoids

In order to identify capsule geometries that outperform the spherical design, several superellipsoids investigated in the parametric study were selected for further investigations with the PBLTESS model described in Section 2.5. The simulations included the two geometries shown in Figure 7 as well as the geometries achieving the highest SVR for packing densities of minimum 58%, 60%, 62%, and 64%. Additionally, a spherical design was included as a reference, which has an average packing density of 64%. The goal was to identify capsules with higher thermal power but a similar packing density, which allows them to store/release more energy during a given time period. All geometries considered for the thermal simulations had a volume of 0.96 L; they are listed in Table 4.

For these geometries, both charging and discharging simulations were performed. The PCM used in the simulations was based on ATS 58 from Axiotherm [35] and had a melting range of 56.4–58 °C and a solidification range of 56.6–54.8 °C. The HTF was water, and the encapsulation material was polypropylene (PP) with a thickness of 1 mm. The simulated storage tank was cylindrical and 1.983 m high, with an inner diameter of 0.784 m. A schematic of the simulated system is shown in Figure 8, while the properties of the HTF and the materials involved are listed in Table 5.

Table 4. Geometries considered for charging and discharging simulations and their corresponding superellipsoid parameters.

Denomination	β	γ	e	n	A_C [m ²]	SVR [m ⁻¹]	ε [%]	Shape
PD58	4	0.7	0.2	1.25	0.0721	75.01	58.22	
PD60	2	0.4	0.2	1.25	0.0644	66.97	61.75	
PD62	0.4	0.4	0.2	1.667	0.0574	59.70	62.84	
PD64	1	0.4	0.2	1	0.0554	57.61	64.32	
PDMax	1	0.7	0.2	1.667	0.0517	53.73	65.22	
SVRMax	1	8	0.2	1.667	0.1385	144.00	37.23	
SPH	1	1	0.2	1	0.0471	48.97	64.00	

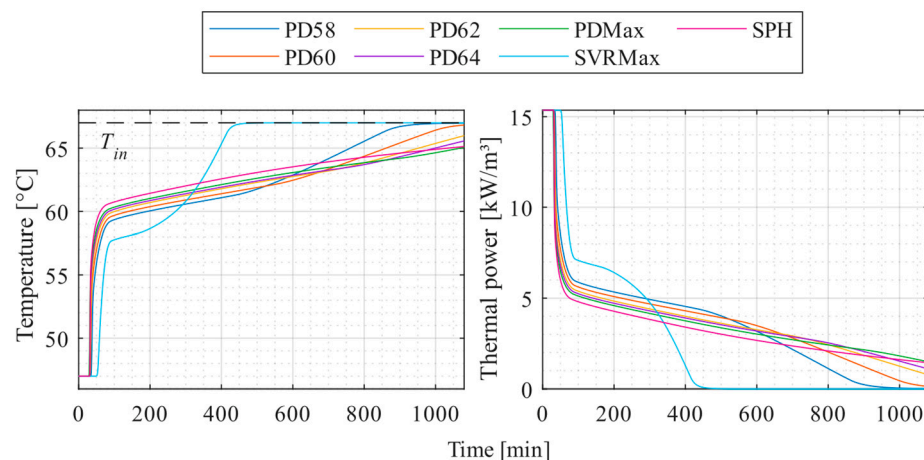
**Figure 8.** Schematic of the simulated PBLTESS.

The mass flow rate used in the simulation study was 600 kg/h, the simulated time was 18 h. The charging process was carried out by feeding HTF at 67 °C from the top, while the initial temperature inside the tank was 47 °C. Vice versa, discharging was performed by feeding HTF at 47 °C from the bottom, while cooling down the tank from its initial temperature of 67 °C.

Table 5. Thermal properties of PCM, encapsulation material and HTF.

Property			ATS 58	PP	Water
Thermal conductivity	solid	[W/mK]	0.4	0.21	-
	liquid		0.35	-	0.65
Density	solid	[kg/m³]	1450	900	-
	liquid		1260	-	984.7
Specific heat capacity	solid	[J/kgK]	2120	1989	-
	liquid		2970	-	4181.8
Latent heat		[kJ/kg]	200	-	-

The results of the charging simulations are shown in Figure 9. With the capsule geometry having the highest SVR, the charging process was completed first, as expected. The other geometries follow according to their respective SVR. Not all geometries completed melting within the simulated time, but the trajectory of the temperature profiles indicates that the charging duration for the spherical design was the longest. The thermal power, which was normalized with respect to the storage tank volume, generally follows the temperature curves. With temperature differences getting smaller, the heat transfer rate between the capsules and the HTF decreases. Since the heat transfer area of the geometries with high SVR is large, their highest power input is during the phase change, albeit for a short period of time. This is particularly true of the SVRMax model, which achieves more than 50% higher thermal power than the spherical design.

**Figure 9.** Results of the charging simulations for the six superellipsoidal and one spherical PCM capsules: outlet temperature (**left**) and normalized thermal power (**right**).

Similar observations can be made regarding the discharging process, which is shown in Figure 10. The superellipsoids with high SVR complete the process earlier than those with high packing densities. Also, the thermal power profiles during charging and discharging appear very similar, which could be expected since the model does not account for specific melting or solidification effects (here mainly subcooling).

In addition, the PCM liquid fraction averaged across all capsules in the packed bed was determined, as it provides insights into the charging state of the PBLTESS. Figure 11 shows the simulated profiles of the liquid fraction for the seven capsule designs considered. The same trends as in the two previous figures can be observed, i.e., the higher the SVR, the quicker the phase change occurs. It becomes clear that the spherical capsule geometry requires a significantly longer time for a complete phase change compared to the other designs. While the phase change process is complete after the simulated time of 18 h for

most other capsule designs, only about half of the PCM volume in the spherical capsules had changed its state. This is due to the low SVR of spheres and represents the reason PCM capsule designs that are based on a sphere are rather unsuitable for PBLTESS.

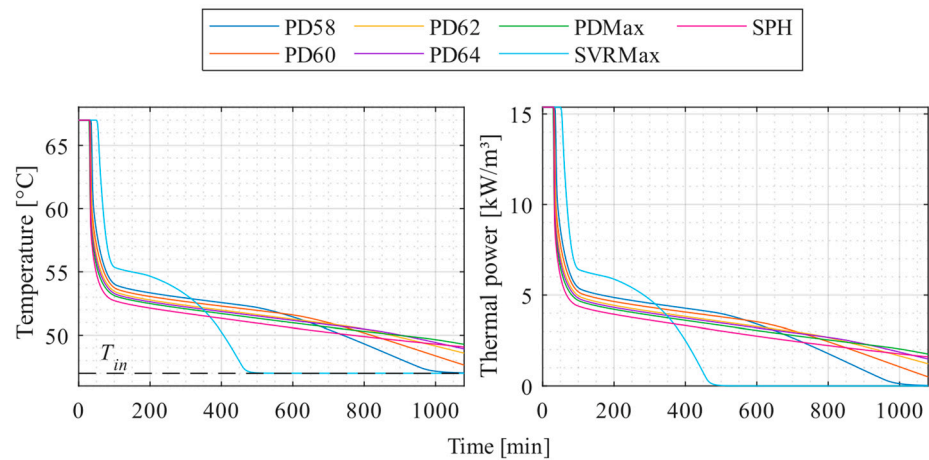


Figure 10. Results of the discharging simulations for the six superellipsoidal and one spherical PCM capsules: outlet temperature (**left**) and normalized thermal power (**right**).

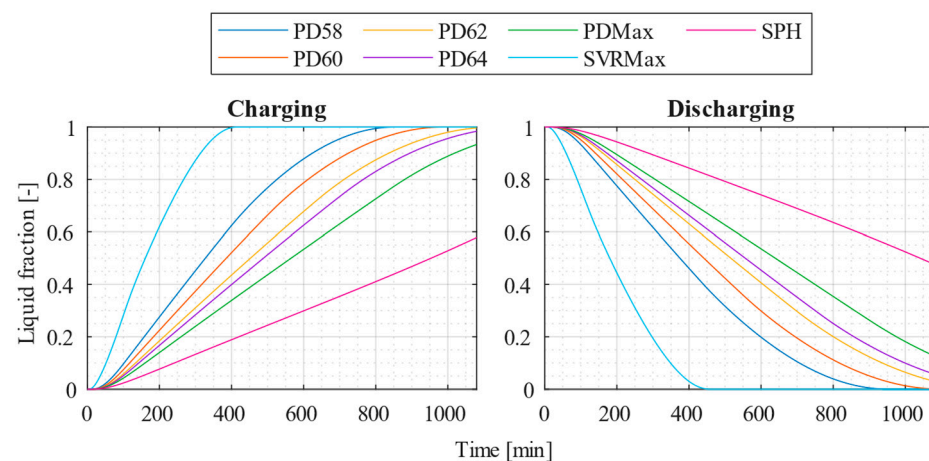


Figure 11. Simulated liquid fraction profiles during charging and discharging using six different superellipsoidal and one spherical PCM capsule design.

The limitations in performance of the spherical capsules become even more apparent when the thermal power is integrated over time, yielding the amount of thermal energy that is released or stored during charging or discharging. In Figure 12, the thermal energy stored/released by the simulated PBLTESS during charging/discharging periods of 4, 8, 12, and 18 h is shown. The spherical design transfers the least amount of energy during these time periods, and, in particular, the utilization of the contained PCM is significantly lower compared to the other designs. Even the capsule variant, which achieves the highest packing density at 65.2%, transfers energy faster than the spherical design, which has a packing density of only 64%. Therefore, an important finding of this study is that PCM capsules with similar packing densities to spheres can have significantly better heat transfer capabilities hence offering an attractive alternative to the state-of-the-art spherical capsules.

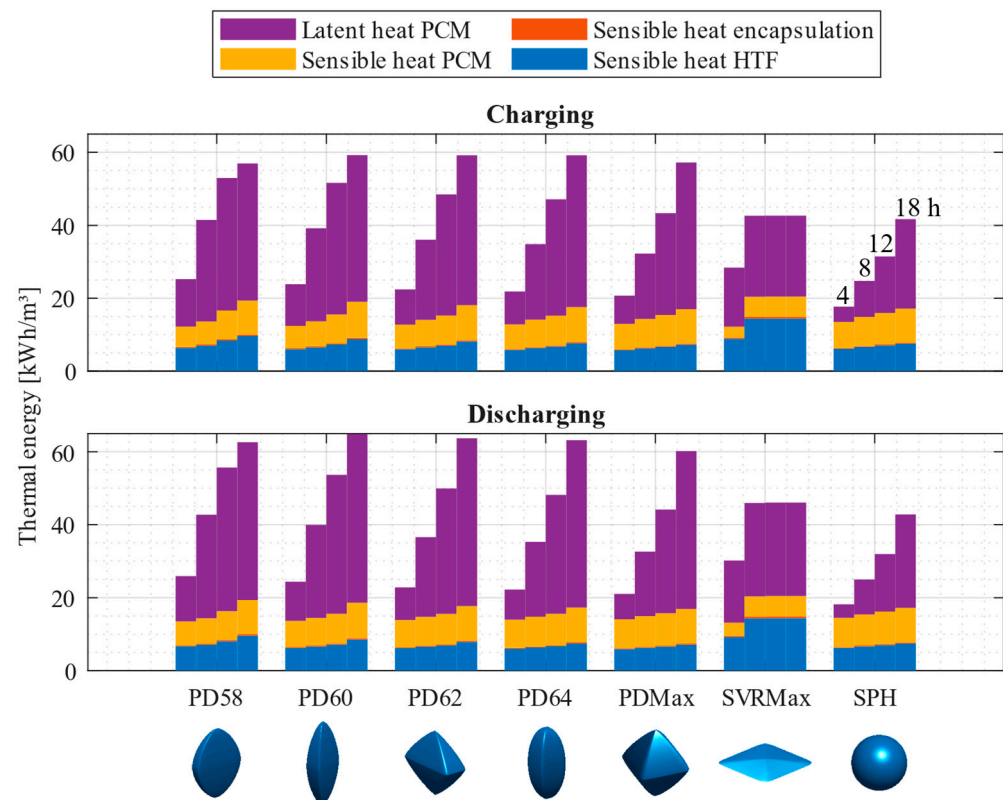


Figure 12. Simulated thermal energy (normalized with respect to storage tank volume) absorbed/released during charging/discharging for seven different PCM capsule designs after 4 h, 8 h, 12 h, and 18 h (represented by the first, second, third and fourth bar in each bar chart group).

The capsule variant with maximum SVR performs quite well during the first four hours and is capable of releasing its stored energy very fast, which corresponds to the high thermal power output shown in Figures 9 and 10. Therefore, this design could be suitable for applications requiring fast charging and discharging rates, such as in back-up cooling or heating systems. The other capsule designs (indicated by PD) show quite similar results. It can be seen that the packed bed with PD58 capsules delivers the best performance for periods of up to twelve hours, while over an 18 h period, the PD60 variant can store or release the largest amount of energy. Ultimately, the PDMax geometry contains the highest amount of energy when a complete charge/discharge cycle is considered. Depending on the charging/discharging duration, the storage capacity of the superellipsoidal PCM capsules exceed that of the spherical design by 15% to 86%.

In general, the optimal capsule design depends primarily on the application and operating conditions. When fast charging and discharging rates, i.e., high thermal power, are required, the SVRMax capsules design appears to be the most suitable solution among the capsule variants evaluated. When high storage capacity is required, the PDMax design seems more appropriate.

As for pressure loss, geometries with high packing density are typically expected to result in higher pressure losses. However, preliminary experimental data suggest that pressure loss is largely attributable to static pressure, since the average flow velocities inside the storage tank are quite low, with Reynolds numbers below 250.

4. Conclusions

In this work, first, a parametric study was carried out, in which different superellipsoid capsule geometries were investigated regarding their packing density and SVR. Superellipsoids were used because they offer great flexibility and versatility in geometry

creation, while requiring only five input parameters. A total of 116 superellipsoids with the same volume were considered. To determine the packing densities, DEM-based bed filling simulations were performed for each geometry and validated based on experimental data yielding an average deviation of less than 5%. The DEM results showed that several superellipsoids achieve higher packing densities than spheres, while they also exhibit higher SVR values. The key results of the parametric study are as follows:

- The geometry with the highest packing density ($\varepsilon = 65.2\%$) among all investigated superellipsoids has the parameter combination $\beta = 1$, $\gamma = 0.7$, $e = 0.2$ and $n = 1.667$.
- The geometry with the highest surface-area-to-volume ratio ($\text{SVR} = 144 \text{ m}^{-1}$) has the parameter combination $\beta = 1$, $\gamma = 8$, $e = 0.2$ and $n = 1.667$.
- When comparing all geometries with a packing density of at least
 - o 58%, geometry PD58 had the highest SVR of 75.01 m^{-1} , a packing density of $\varepsilon = 58.22\%$ and the parameter combination $\beta = 4$, $\gamma = 0.7$, $e = 0.2$, $n = 1.25$.
 - o 60%, geometry PD60 had the highest SVR of 66.97 m^{-1} , a packing density of $\varepsilon = 61.75\%$ and the parameter combination $\beta = 2$, $\gamma = 0.4$, $e = 0.2$, $n = 1.25$.
 - o 62%, geometry PD62 had the highest SVR of 59.70 m^{-1} , a packing density of $\varepsilon = 62.84\%$ and the parameter combination $\beta = 0.4$, $\gamma = 0.4$, $e = 0.2$, $n = 1.667$.
 - o 64%, geometry PD64 had the highest SVR of 57.61 m^{-1} , a packing density of $\varepsilon = 64.32\%$ and the parameter combination $\beta = 1$, $\gamma = 0.4$, $e = 0.2$, $n = 1$.

In general, the influence of the aspect ratios on the packing densities seems to be greater than that of the varied shape factor. Also, SVR and packing density seem to be in an inversely proportional relationship, i.e., a high SVR typically leads to a low packing density and vice versa.

After analyzing the DEM simulation results, a thermal 1D PBLTESS model was used to evaluate six selected superellipsoidal capsule designs (PDMax, SVRMax, PD58, PD60, PD62, PD64) by comparing their performance to that of a spherical capsule design. These simulations showed that higher packing densities lead to longer charging and discharging durations, while these durations were shorter at higher SVR values. Furthermore, the sphere proved inferior to all of the considered superellipsoidal geometries. In fact, the storage capacity of superellipsoidal PCM capsules could exceed the capacity of the spherical design by 15% to 86% depending on the charging/discharging duration. These results demonstrate a clear incentive for the use of non-spherical PCM capsules in PBLTESS.

The optimal capsule design generally depends on the desired application and its operating conditions. When high thermal power output is required such as in back-up cooling or heating system, the SVRMax design seems to be the most suitable solution among the geometries considered. When high storage capacity is required, such as in seasonal storage systems, the PDMax design appears to be more appropriate.

Future work includes generalizing the superellipsoidal packing properties by using Design of Experiment methods to determine functional relationships between the geometrical parameters and packing density and SVR, respectively. Additionally, a PCM capsule prototype of one of the designs described in Section 3.2 is currently in production and will be experimentally tested to generate additional validation data for the PBLTESS model.

Author Contributions: Conceptualization, M.G. and E.Y.K.; methodology, M.G. and L.K.; software, M.G. and L.K.; validation, M.G. and L.K.; formal analysis, M.G. and L.K.; writing—original draft preparation, M.G.; writing—review and editing, E.Y.K.; visualization, M.G. and L.K.; supervision, E.Y.K.; project administration, M.G.; funding acquisition, M.G. and E.Y.K. All authors have read and agreed to the published version of the manuscript.

Funding: This research was funded by the German Federal Ministry for Economic Affairs and Energy, grant number 03EN1009F.

Data Availability Statement: The data supporting the conclusions of this article will be made available by the authors on request.

Acknowledgments: We acknowledge support for the publication costs by the Open Access Publication Fund of Paderborn University. Parts of this article were taken from the first author's doctoral dissertation (see Ref. [36]), which can be accessed via Paderborn University Library at <https://digital.ub.uni-paderborn.de/doi/10.17619/UNIPB/1-2199> (accessed on 7 April 2026).

Conflicts of Interest: The authors declare no conflicts of interest. The funders had no role in the design of the study, in the collection, analyses, or interpretation of data, in the writing of the manuscript or in the decision to publish the results.

Abbreviations

The following abbreviations are used in this work:

DEM	Discrete element method
HTF	Heat transfer fluid
LTESS	Latent thermal energy storage system
PBLTESS	Packed bed latent thermal energy storage system
PCM	Phase change material
PP	Polypropylene
SVR	Surface-area-to-volume ratio

References

1. International Energy Agency. Renewables 2025. Available online: <https://www.iea.org/reports/renewables-2025/renewable-heat> (accessed on 22 February 2026).
2. Sarbu, I.; Sebarchievici, C. A Comprehensive Review of Thermal Energy Storage. *Sustainability* **2018**, *10*, 191. [CrossRef]
3. Scheffler, F. Thermische Energiespeicher-Trends, Entwicklungen und Herausforderungen. *Chem. Ing. Tech.* **2019**, *91*, 1219–1228. [CrossRef]
4. Tawalbeh, M.; Khan, H.A.; Al-Othman, A.; Almomani, F.; Ajith, S. A comprehensive review on the recent advances in materials for thermal energy storage applications. *Int. J. Thermofluids* **2023**, *18*, 100326. [CrossRef]
5. Regin, A.F.; Solanki, S.C.; Saini, J.S. Heat transfer characteristics of thermal energy storage system using PCM capsules: A review. *Renew. Sustain. Energy Rev.* **2008**, *12*, 2438–2458. [CrossRef]
6. de Gracia, A.; Cabeza, L.F. Numerical simulation of a PCM packed bed system: A review. *Renew. Sustain. Energy Rev.* **2017**, *69*, 1055–1063. [CrossRef]
7. Mawire, A.; Lefenya, T.M.; Ekwomadu, C.S.; Lentswe, K.A.; Shobo, A.B. Performance comparison of medium temperature domestic packed bed latent heat storage systems. *Renew. Energy* **2020**, *146*, 1897–1906. [CrossRef]
8. Alptekin, E.; Ezan, M.A. A systematic assessment on a solar collector integrated packed-bed single/multi-layered latent heat thermal energy storage system. *J. Energy Storage* **2021**, *37*, 102410. [CrossRef]
9. Suresh, C.; Saini, R.P. Experimental study on combined sensible-latent heat storage system for different volume fractions of PCM. *Sol. Energy* **2020**, *212*, 282–296. [CrossRef]
10. Ismail, K.; Henríquez, J.R. Numerical and experimental study of spherical capsules packed bed latent heat storage system. *Appl. Therm. Eng.* **2002**, *22*, 1705–1716. [CrossRef]
11. Wu, M.; Xu, C.; He, Y.-L. Dynamic thermal performance analysis of a molten-salt packed-bed thermal energy storage system using PCM capsules. *Appl. Energy* **2014**, *121*, 184–195. [CrossRef]
12. Wang, W.; Shuai, Y.; He, X.; Hou, Y.; Qiu, J.; Huang, Y. Influence of tank-to-particle diameter ratio on thermal storage performance of random packed-bed with spherical macro-encapsulated phase change materials. *Energy* **2023**, *282*, 128779. [CrossRef]
13. He, X.; Qiu, J.; Wang, W.; Hou, Y.; Ayyub, M.; Shuai, Y. Optimization design and performance investigation on the cascaded packed-bed thermal energy storage system with spherical capsules. *Appl. Therm. Eng.* **2023**, *225*, 120241. [CrossRef]
14. Cui, J.; Yang, X.; Chen, J.; Wang, P.; Xie, J. Experimental analysis and comprehensive performance improvement research on composite phase change materials packed bed thermal storage systems. *Energy* **2025**, *337*, 138728. [CrossRef]
15. Tao, Y.B.; He, Y.-L. A review of phase change material and performance enhancement method for latent heat storage system. *Renew. Sustain. Energy Rev.* **2018**, *93*, 245–259. [CrossRef]
16. Mehling, H.; Cabeza, L.F. *Heat and Cold Storage with PCM: An up to Date Introduction into Basics and Applications*; Springer: Berlin/Heidelberg, Germany, 2008; ISBN 978-3-540-68557-9.

17. Torquato, S.; Truskett, T.M.; Debenedetti, P.G. Is random close packing of spheres well defined? *Phys. Rev. Lett.* **2000**, *84*, 2064–2067. [CrossRef] [PubMed]
18. Awasthi, A.; Kumar, B.; Nguyen, H.H.; Lee, S.S.; Chung, J.D. Effect of sinusoidal cylindrical surface of PCM on melting performance. *J. Mech. Sci. Technol.* **2020**, *34*, 3395–3402. [CrossRef]
19. Cheng, X.; Zhai, X. Thermal performance analysis of a novel PCM capsule in red blood cell shape. *Appl. Therm. Eng.* **2017**, *120*, 130–137. [CrossRef]
20. Heinz, A.; Moser, C. Numerical modelling and experimental testing of a thermal storage system with non-spherical macro-encapsulated phase change material modules. *J. Energy Storage* **2023**, *58*, 106427. [CrossRef]
21. Axiotherm GmbH. HeatSels®. Available online: <https://www.axiotherm.de/de/produkte/heatsels%C2%AE/> (accessed on 15 March 2026).
22. Jia, H.; Tian, Y.; Tian, X.; Yang, J.; Wang, Q. Numerical investigation on flow characteristics and thermal performance of phase change material in spherical capsules with smooth or dimpled surfaces. *Therm. Sci. Eng. Prog.* **2024**, *50*, 102536. [CrossRef]
23. Sponagle, B.; Maranda, S.; Delgado-Diaz, W.; Waser, R.; Groulx, D.; Worlitschek, J. Experimental validation of a novel modelling technique for packed bed thermal storage systems containing non-spherical phase change material capsules. *Int. J. Heat Mass Transf.* **2025**, *242*, 126794. [CrossRef]
24. Grabo, M.; Acar, E.; Kenig, E.Y. Modeling and Improvement of a Packed Bed Latent Heat Storage Filled with Non-Spherical Encapsulated PCM-Elements. *Renew. Energy* **2021**, *173*, 1087–1097. [CrossRef]
25. Abramowitz, M.; Stegun, I.A. (Eds.) *Handbook of Mathematical Functions: With Formulas, Graphs and Mathematical Tables; Unabridged and Unaltered Republication of the 1964 Edition*; Dover Publications: New York, NY, USA, 1965; ISBN 978-0-486-61272-0.
26. Feng, Y.T.; Han, K.; Owen, D. Energy-conserving contact interaction models for arbitrarily shaped discrete elements. *Comput. Methods Appl. Mech. Eng.* **2012**, *205*, 169–177. [CrossRef]
27. Cundall, P.A.; Strack, O.D.L. A discrete numerical model for granular assemblies. *Géotechnique* **1979**, *29*, 47–65. [CrossRef]
28. Delaney, G.W.; Cleary, P.W. The packing properties of superellipsoids. *Europhys. Lett.* **2010**, *89*, 34002. [CrossRef]
29. Zhao, S.; Zhang, N.; Zhou, X.; Zhang, L. Particle shape effects on fabric of granular random packing. *Powder Technol.* **2017**, *310*, 175–186. [CrossRef]
30. Ismail, K.; Stuginsky, R., Jr. A parametric study on possible fixed bed models for pcm and sensible heat storage. *Appl. Therm. Eng.* **1999**, *19*, 757–788. [CrossRef]
31. Churchill, S.W. A comprehensive correlating equation for laminar, assisting, forced and free convection. *AIChE J.* **1977**, *23*, 10–16. [CrossRef]
32. Gnielinski, V. Berechnung des Wärme- und Stoffaustauschs in durchströmten ruhenden Schüttungen. *Verfahrenstechnik* **1982**, *16*, 36–39.
33. Gnielinski, V. G9 Wärmeübertragung bei erzwungener Konvektion: Durchströmte Haufwerke. In *VDI-Wärmeatlas*; Stephan, P., Kabelac, S., Kind, M., Mewes, D., Schaber, K., Wetzel, T., Eds.; Springer: Berlin/Heidelberg, Germany, 2019; pp. 889–891. ISBN 978-3-662-52988-1.
34. Kast, W.; Krischer, O.; Reinicke, H.; Wintermantel, K. *Konvektive Wärme und Stoffübertragung*; Springer: Berlin/Heidelberg, Germany, 1974; ISBN 978-3-540-06384-1.
35. Axiotherm GmbH. ATS 58: Data Sheet. Available online: <https://www.axiotherm.de/de/produkte/axiotherm-pcm/> (accessed on 8 April 2026).
36. Grabo, M. Modeling and Optimization of Energy System Components Equipped with Phase Change Materials. Ph.D. Thesis, Universitätsbibliothek, Paderborn, Germany, 2025. [CrossRef]

Disclaimer/Publisher’s Note: The statements, opinions and data contained in all publications are solely those of the individual author(s) and contributor(s) and not of MDPI and/or the editor(s). MDPI and/or the editor(s) disclaim responsibility for any injury to people or property resulting from any ideas, methods, instructions or products referred to in the content.