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▶ To cite this version:

A. El Ouali, Y. Khattari, B. Lamrani, T. El Rhafiki, Y. Zeraouli, et al.. Apparent heat capacity method to describe the thermal performances of a latent thermal storage system during discharge period. Journal of Energy Storage, 2022, 52, pp.104960. 10.1016/j.est.2022.104960. hal-04088403

HAL Id: hal-04088403 https://hal.science/hal-04088403v1

Submitted on 22 Jul 2024

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Apparent heat capacity method to describe the thermal performances of a latent thermal storage system during discharge period

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Abstract:

In this work, a novel detailed dynamic model for latent cold thermal storage unit containing water as phase change material (PCM) is presented. The proposed dynamic model is based on transient energy balances for both PCM capsules and heat transfer fluid (HTF). The apparent heat capacity approach is used to model phase transition processes in PCM, where the PCM heat capacity is given as a temperature-dependent function. This method can be simply integrated into a variety of software to assess the energy efficiency of latent storage. The dynamic model of the PCM storage unit is validated using measured results from the literature and it is used to investigate the influence of multiple parameters on the storage thermal performance. The obtained result show that the PCM melting process varies in both axial direction and radial direction in the storage unit. It was also observed that the higher the height of the tank, the longer the discharge period. Increasing the diameter of capsules from 47 mm to 77 mm leads to increase the discharging period by about 30 %. In addition, varying the storage tank initial temperature between -8 $^{\circ}$ C to – 4 $^{\circ}$ C does not have a significant effect of on the discharging time. Finally, it was recommended that for improving the storage performance and minimizing water pumper energy consumption, a compromise between the HTF flow rate and the capsule diameter must be determined.

Keywords: Latent storage system; cold storage; PCM; Apparent heat capacity; Packed bed; Heat transfer.

Nomenclature

A_{f}	specific surface of the capsule (m-1)
ср	specific heat (J.kg ⁻¹ .K ⁻¹)
d	diameter (m)
Н	height tank (m)
Lf	latent heat (J.kg ⁻¹)
Pr	Prandtl number
q_v	flow rate $(m^3.h^{-1})$
r	rayon (m)
Ra	Rayleigh number
Re	Reynolds number
t	time (s)
Т	temperature (°C)
u	velocity (m.s ⁻¹)
U_{f}	convective transfer coefficient $(W.m^{-2}.K^{-1})$
Х	position along the direction of the tank (m)

Greek letters

β	liquid fraction
ρ	density (kg.m ⁻³)
μ	dynamic viscosity (Pa.s ⁻¹)
λ	thermal conductivity (W.m ⁻¹ .K ⁻¹)
ε	porosity
Subscripts	
App	apparent
HTF	heat transfer fluid
f	fluid
1	liquid
m	melting
PCM	phase change material
S	solid

1. Introduction

Thermal storage systems using phase change materials are presently used in several industrial applications [1] such as waste heat recovery [2], industrial cold [3-4], HVAC [5], district heating [6-7], thermal management of electronic devices and batteries [8-9]. Such systems are considered indispensable to support the energy transition and manage the intermittency of renewable energies [10-12].Thermal storage systems using phase change materials (PCMs) are advantageous as they allow thermal energy to be stored close to their melting temperature in a specified storage volume [13]. When demand for thermal energy is lower than production, the latent thermal storage system stores the unused thermal energy. On the other hand, during periods of peak consumption, the thermal storage system releases the accumulated thermal energy [14-15].

Usually, PCM is enclosed in capsules, which can be spherical, cylindrical or rectangular [16-17]. Other geometries are under development such as biomimetic red blood cell (RBC) shaped capsules for thermal storage of latent heat. The RBC shape offers a considerably higher heat transfer rate than other shapes [11-12]. However, research is underway to characterize the heat transfer between these capsules and the heat transfer fluid in the storage tanks [11-12].

Spherical capsules are widely used for industrial applications [18-20]. Using this geometry, the heat transfer surface between the heat transfer fluid (HTF) and the PCM can be enhanced. Several studies have been carried out on the numerical analysis and physical modeling of the transition process inside a tank filled with PCMs enclosed in spherical capsules [21]. The thermal performance of a latent storage system has been evaluated using different physical models such as the homogeneous model [22-23], the Schumann model [24-26], the continuous solid phase model [27-32] and the concentric diffusion model [33-38]. All of these models consider that the packed bed system acts as a porous medium [21]. The homogeneous model is rarely used as the assumption of a single local temperature for both solid and liquid media is only valid if the PCM capsule have a conductivity close to that of the fluid or when they have a small diameter [39]. Schumann's model ignores the thermal conduction inside the particle. However, when the thermal conductivity of the PCM is low (which is the majority of cases) or when the particle size is high, then the internal thermal resistance cannot be neglected [40]. The continuous solid phase model considers PCM capsules as a continuous medium and not as a medium composed of independent spherical capsules. Therefore, the internal thermal conduction in the particle is not taken into account. On the other hand, the conduction in the axial (one-dimensional model) direction is considered [31-32]. The concentric diffusion model is a heterogeneous two-phase model that has the characteristic of considering the thermal conduction inside the PCM capsules. As the shape of the capsules is spherical, the thermal conduction is radial [41-42]. This model is indeed the only one taking into account the radial heat conduction within the PCM, even if it increases considerably the computation time. The thermal radial conduction is important especially when the flow rate is low [43-47]. As an example, Peng et al. [46] studied the comportment of a PCM capsules inside the tank. The transition process within the PCM is analysed using the enthalpic method. The results obtained are validated with the experimental results of Izquierdo-Barrientos et al. [47]. The authors [47] indicate that decreasing the size of the PCM capsule or the fluid inlet velocity, or increasing the bed height increase the thermal efficiency of the system. Tafone et al. [48] adopted the concentric diffusion model to investigate the packed bed contained spherical PCM capsules for liquid air energy storage system. The apparent heat capacity approach was adopted to address the phase transition inside the capsule. The same model was also employed by Li et al. [49-50] to address the thermal performance of a latent storage system containing PCM confined in spherical capsules. The authors [49-50] indicate that the performance of the system can be improved by the HTF inlet temperature and the mass flow rate of the latter. They also showed that a smaller capsule diameter results in better system performance and that an increase in the size of the capsules leads to an increase in the melting process time. It is important to note that in most of the studies using the concentric diffusion model, authors present only the evolution of the HTF temperature in the packed bed. To the best of the authors' knowledge, the evolution of the temperature within the PCM as a function of the spherical capsule radius during the discharge period has not been reported in any of the previously mentioned papers.

The expression of heat capacity and enthalpy of PCM as a function of temperature during the phase transition process is essential for correct mathematical modelling of heat transfer inside the spherical capsules. However, when the physical model is derived from the apparent capacity approach, the heat transfer inside the PCM can be described by a single energy equation. This simplifies the mathematical resolution of the differential equations that describe the flow and heat transfer in the latent storage tanks. Our original contribution in this work lies in the following main points:

• A physical model based on the apparent heat capacity approach has been developed to investigate the thermal performances of the packed bed. The physical model was then validated based on experimental results from the literature.

- We propose a complementary analysis of the phase transition inside the capsules at different positions in the tank.
- The influence of different parameters on the thermal performance of the tank has also been highlighted.

2. Physical model

Fig.1 illustrates the Latent Storage System used in this study. It consists of a cylindrical tank with a height L and a diameter d_t . The tank contains a PCM confined in spherical capsules placed randomly with a porosity \mathcal{E} . The capsules have a diameter d_{pcm} and are made of high polyethylene density. During the charging/discharging process, the heat transfer fluid (HTF) moves in at a constant temperature from the bottom of the tank to give up/accumulate heat by convective transfer. HTF used in our study will be water. The charging/discharging process is considered complete when the temperature becomes uniform on the whole system. The main parameters of our storage system are summarised in **Table 1**.



Fig.1: Latent storage system

Parameters	Valuer
Tank height (H) [m]	1, 1.42, 2
Tank diameter (dt) [m]	0.95
Capsule diameter (d _{pcm}) [mm]	47, 67, 77
Porosity (\mathcal{E})	0.4
HTF flow rate $(q_v) [m^3.h^{-1}]$	1, 1.5, 2.3, 2.6, 3
HTF initial temperature [°C]	-4, -6, -8

 Table 1: Main parameters of the storage tank

Before describing the physical model, it is fundamental to specify the main assumptions:

- The tank is assumed to be perfectly insulated.
- The flow of the HTF is monodirectional from the bottom to the top.
- Heat conduction in the spherical capsules occurs radially (i.e. constrained melting).
- The spherical capsules are considered as an isotropic porous medium.
- The packed bed is divided it into several layers in the axial direction. All the spheres of the same layer are assumed to act similarly and each layer can be modelled and discretized using a single sphere.

The system of energy conservation equations consists of two coupled expressions: one equation for the HTF and another for PCM. By considering the previously mentioned assumptions, the equations of the model are the following:

For HTF:

$$\rho_{f}c_{f}\varepsilon\frac{\partial T_{f}}{\partial t} + \varepsilon\rho_{f}c_{f}u_{f}\frac{\partial T_{f}(x,t)}{\partial x} = \varepsilon\lambda_{f}\frac{\partial^{2}T_{f}(x,t)}{\partial x^{2}} + U_{f}A_{f}\left(T_{pcm}(r=\frac{d}{2}) - T_{f}(x,t)\right)$$
(1)

> For PCM:

(2)

$$\rho_{pcm}c_{pcm}\frac{\partial T_{pcm}(r,t)}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\lambda_{pcm}\frac{\partial T_{pcm}(r,t)}{\partial r}\right)$$

where, T_f and T_{pcm} indicate the HTF and PCM temperature respectively, u_f is the HTF velocity, c_f is the specific heat capacity of the HTF, c_{pcm} is the apparent heat capacity of the PCM, ρ_f is the HTF density, ρ_{pcm} is the PCM density, λ_f is the thermal conductivity of HTF, λ_{pcm} is the thermal conductivity of PCM and \mathcal{E} is the porosity of the packed bed. The coefficient A_f is the specific surface of the capsule per unit volume and is expressed as follows:

$$A_f = \frac{6(1-\varepsilon)}{d_{capsule}}$$
(3)

The convective transfer coefficient U_f between the HTF and the capsules is defined by [51]:

$$U_{f} = \frac{\lambda_{f}}{d} \Big[3.22 \,\mathrm{Re}^{1/3} \,\mathrm{Pr}^{1/3} + 0.117 \,\mathrm{Re}^{0.8} \,\mathrm{Pr}^{0.8} \Big]$$
(4)

The Reynolds and Prandtl numbers can be written as follows:

$$\operatorname{Re} = \frac{\rho_f d_{capsule} \mathcal{E} u_f}{\mu_f}$$
(5)

$$\Pr = \frac{c_{p,f}\mu_f}{\lambda_f}$$
(6)

When the physical model is derived from the apparent capacity approach, the heat transfer inside the PCM can be described by a single energy equation. This makes it easier to solve the differential equations that describe the flow and heat transfer in storage tanks properly. In our case, the apparent heat capacity and the thermal conductivity of the PCM is calculated by using the following expressions [52][9]:

$$c_{pcm} = \beta c_{pcm,l} + (1 - \beta) c_{pcm,s} + L_f \frac{\frac{2\gamma}{\Delta T}}{\pi \left[\left(\left(T - T_m \right) \left(\frac{2\gamma}{\Delta T} \right) \right)^2 + 1 \right]}$$
(7)

where $c_{pcm,l}$ and $c_{pcm,s}$ are the specific heat capacity of PCM in solid and liquid states, ΔT is the width of the melting phase temperature, and T_m is the melting temperature of the PCM. β is the liquid fraction which can be calculated by the following expression [52]:

$$\beta = \frac{1}{2} \left[\tanh\left[\frac{2\gamma(T - T_m)}{\Delta T}\right] + 1 \right]$$
(8)

Furthermore, our physical model also needs to consider the variation of the PCM thermophysical properties during phase transition:

$$\rho_{pcm} = \beta \rho_{pcm,l} + (1 - \beta) \rho_{pcm,s}$$
(9) $\lambda_{pcm} = \beta \lambda_{pcm,l} + (1 - \beta) \lambda_{pcm,s}^{eff}$

where $\lambda_{pcm,s}$ and $\lambda_{pcm,l}^{eff}$ are thermal conductivities of PCMs in solid and liquid states and $\rho_{pcm,s}$ and $\rho_{pcm,l}$ are densities of PCM in solid and liquid states.

During constrained melting, heat conduction acts only at the initial stage of the melting process. This leads to a nearly concentric melting of the PCM inside the spherical capsule **[53]**. During the melting process, an oval shape emerges in the upper part of the solid PCM, but the profile of the lower part remains relatively unchanged. The oval shape is caused by natural convection as the liquid layer increases **[54]**. Natural convection occurs because the hot liquid in the PCM rises while the cooler liquid flows down to replace the hotter fluid. This creates an unsteady fluid flow inside the capsule, known as buoyancy-driven convection. The top part of the solid PCM melts faster than the bottom part. Natural convection also occurs in the lower half of the spherical capsule, resulting in the wavy profile of the lower part of the solid PCM **[55]**. In our physical model, the correlation suggested by Lacroix **[56]** is chosen to evaluate the effective thermal conductivity by including the natural convection occurring during the fusion process:

$$\lambda_{eff,pcm}^{l} = a.Ra^{b}.\lambda_{pcm}^{l}$$
(10-b)

where, *a* and *b* are constants and equal to 0.05 and 0.5, respectively. The Rayleigh number Ra is computed using the following expression:

$$Ra = \left(\beta g\left(\rho c\right)_{pcm}^{l} d^{3} \left|T_{f} - T_{m}\right| / \left(\mu_{pcm}^{l} \lambda_{pcm}^{l}\right)\right)$$
(10-c)

where, g is the gravitational acceleration, β is the PCM thermal expansion coefficient and μ_{pcm}^{l} is the dynamic viscosity of the liquid PCM.

The initial and boundary conditions of the latent storage system are:

 $t = 0; \forall x; \forall r$ $T_{f}(x, t = 0) = T_{pcm}(r, t = 0) = T_{ini}$ (11) x = 0; t > 0 $T_{f}(x, t) = T_{f, inlet}$ (12) x = L; t > 0 $\frac{\partial T_{f}(x = L, t)}{\partial x} = 0$ (13) r = 0; t > 0 $\frac{\partial T_{pcm}(r = 0, t)}{\partial r} = 0$ (14)
At the capsule wall:

$$r = r_0; t > 0 \qquad \qquad -\lambda_{pcm} \frac{\partial T_{pcm}(\mathbf{r} = r_0, t)}{\partial r} = U_f \left(T_{pcm, r = r_0} - T_f \right)$$

(14)

3. Numerical method

The fully implicit finite volume method was implemented to solve the system of energy equations. The first-order upwind scheme was used to address the convection terms, and the diffusion terms are discretized employing the second-order central differential scheme. Accordingly, the resulting energy equation system can be written as follows:

> HTF

$$a_{f,P}T_{f,P} = a_{f,W}T_{f,W} + a_{f,E}T_{f,E} + a_{f,P}^0T_{f,P}^0 + b_f$$
(15)

With :

$$a_{f,P} = a_{f,W} + a_{f,E} + U_f A_f \Delta x$$
(16)

$$a_{f,W} = \frac{\varepsilon \lambda_f}{\Delta x} + \varepsilon \rho_f c_f \frac{u}{2}; a_{f,E} = \frac{\varepsilon \lambda_f}{\Delta x} - \varepsilon \rho_f c_f \frac{u_f}{2}; b_f = U_f A_f T_{pcm} \left(\mathbf{r}_0, t \right)$$
(17)

$$a_{pcm,P}T_{pcm,P} = a_{pcm,W}T_{pcm,W} + a_{pcm,E}T_{pcm,E} + a_{pcm,P}^{0}T_{pcm,P}^{0}$$
(18)

With :

$$a_{pcm,P} = a_{pcm,P}^{0} + a_{pcm,W} + a_{pcm,E}$$
(19)

$$a_{pcm}^{0} = \rho_{pcm} c_{pcm} \left(\frac{r_{E}^{2} - r_{W}^{2}}{3\Delta t} \right); a_{pcm,W} = \frac{r_{W}^{2} \lambda_{pcm,W}}{\Delta r}; a_{pcm,E} = \frac{r_{E}^{2} \lambda_{pcm,E}}{\Delta r}$$
(20)

where *E* and *W* are the East and West of each control volume. r_E and r_W refer to the local radius of the P control volume faces. In this work, equations **15** and **18** were solved iteratively using a tridiagonal matrix algorithm (TDMA) method [**57**]. The computational process was carried out using Fortan 90. The iteration that was specified in each time interval was considered convergent when the maximum relative residual of T_f and T_{pcm} was less than 10⁻⁴.

4. Model validation

Before reporting, the results related to our study, it is necessary to verify our numerical model. For this purpose, experimental results presented by Bedecarrats et al. [58] are relied

on. In their study, Bedecarrats et al. [58] presented experimental results during the fusion phase inside a tank charged with a spherical capsule enclosing water as a PCM (see **Table 2**). The latent storage system is a cylinder with a height of 1.42 m and a diameter of 0.95 m. Polyurethane foam was employed to insulate the tank thermally. The capsules are filled with water as PCM and are 77 mm in diameter. At the initial instant, the tank temperature (HTF (glycol water) and PCM) is equal to -6°C. The PCM, in that case, is in the solid state (ice). During the discharge period, the HTF flows in the storage tank from the top to the bottom. The HTF temperature at the entry of the tank increases progressively during the first hours to reach a final temperature (T_s) of about +6°C.

Density (kg.m ⁻³)		
Solid		
Liquid		
Latent heat (kJ.kg ⁻¹)	333	
Melting temperature (°C)	0	
Specific heat capacity (J.kg ⁻¹ .°K ⁻¹)		
Solid 2040		
Liquid 4220		
Thermal conductivity (W.m ⁻¹ .K ⁻¹)		
Solid 2.25		
Liquid 0.6		

Table 2: Main properties of water

It's worth noting that the phase transition happens outside of the melting temperature during the charge phase (crystallisation). A delay in the crystallization is often due to the presence of the supercooling phenomenon [59-60]. This phenomenon can be simulated using the nucleation laws [59-60]. In the following, numerical simulations will be carried out during the discharge period (i.e. melting process), based on a tank initially considered at the initial temperature T_i . We assumed that the moment when the HTF temperature at the outlet of the

tank reaches that of the inlet corresponds to the end of the discharge process. Several simulations were performed to illustrate the effect of HTF flow rate, capsules diameter, tank height and the initial temperature of the system.

The comparison between the experiment and numerical model is presented in **Fig.2-a** through the variation of the HTF temperature at the exit of the tank versus time for various flow rates. The numerical results seem to be in close accord with the experimental ones, thus allowing the validation of the model (see **Fig.2-a**). As shown in this plot, the higher the HTF flow rate, the lower the discharge time. As the HTF flow rate increases, the heat transfer coefficient between capsules and HTF increases. For the three HTF flow rates considered, all the thermal latent energy of the PCM has been recovered by the HTF.



Fig.2-a: HTF temperature versus time at the exit of the system for various flow rates.

We consider that a significant increase in the flow rate does not necessarily imply a significant effect on the discharge time. Moreover, this leads us to think that there would be a limit value of the HTF flow rate, beyond which the discharge time would not decrease anymore (see Fig.2-b).



Fig.2-b: Effect of the HTF flow rate on the discharge duration

It is important to note that Bedecarrats et al. [59] and Kousksou et al. [60] have also developed a physical model of this system by taking into account the thermal conduction in the PCM. In their paper, the authors report only the HTF temperature evolution inside the packed bed. The PCM temperature variation along the radius of the capsules and across the storage tank has not been mentioned in their work [59-60].

In **Fig.3**, we presented the evolution of the HTF temperature between the inlet and the outlet of the tank. The capsule diameter is 77 mm and the tank height is 1.42 m. This graph shows clearly that the fluid flow in the tank is stratified and piston flow.



Fig.3: HTF temperature versus time for various positions inside the tank

5. Results and discussion

The physical model is now used to determine the PCM temperature evolution within the capsules for different locations in the tank (see **Fig.4**). We notice that the time of PCM melting in capsules located at the inlet of the tank is shorter than that of capsules situated at the outlet of the tank. Similar tendancies have been found by other authors for a storage tank using other phase change materials [49-50]. The curves also indicate that the temperature gradient in the capsules decreases between the inlet and outlet of the tank. Such results can be attributed to the higher HTF temperature level at the tank inlet compared to that at the tank outlet. This helps to enhance the heat transfer between the HTF and the PCM and accelerate the melting process inside the capsules. In fact, the phase change process leads to a sudden variation and discontinuities in thermodynamic properties. This renders the mathematical modeling of the phase transition more challenging **[61-62]**. However, the results obtained indicate that the phase change of the PCM (i.e. ice) is not occurring at 0°C, but over a range of temperature. This is due to the apparent capacity approach, which was employed in the present work to simulate the melting process in the capsules.



(a) Tank inlet (b) Middle of the tank



(c) Tank outlet

Fig.4: PCM temperature evolution within the capsules at different locations in the tank

In addition, the physical model permits to determine the evolution of the global liquid fraction of the PCM inside the tank, which allows identifying the end of the latent discharge process (see **Fig.5**). It should be noted that the liquid fraction varies between 0 and 1, when the PCM temperature is around its melting temperature T_m , e.g. within the temperature range of the

phase transition $T_m - \frac{\Delta T}{2}$ and $T_m + \frac{\Delta T}{2}$. Below or above the temperature range, the value of the liquid fraction become 0 or 1, respectively. In general, the liquid fraction inside each capsule can be presented in the simulation by either straight line temperature-dependent discontinuous functions using conditional statements [63] or simplified temperature-dependent continuous functions [62]. However, a number of researchers [62-64] have noted that using discontinuous functions increases the computational time of simulation.



Fig.5: Global liquid fraction of the PCM versus time

The influence of the capsule diameter on the thermal performance of the tank was examined and presented in **Fig.6**. Three diameters were considered: $d_{pcm} = 44$ mm; $d_{pcm} = 64$ mm and $d_{pcm} = 77$ mm. We observe that as the capsule diameter decreases, the discharge time is reduced. Reducing the capsule diameter results in an increase in the number of capsules and consequently the area of exchange between the PCM capsules and the HTF. For the three diameters considered, all the latent thermal energy due to the melting has been recovered by the HTF.



Fig.6: HTF temperature at the tank outlet versus time for various capsule diameter

The PCM temperature profile inside the capsules for the three diameters in the middle of the tank has been indicated in **Fig.7**. We note that for the same flow rate and at the same position in the tank, the thermal gradient within the capsules rises as the capsule diameter increases. These plots also confirm that the duration of the phase change within the capsules diminishes as the capsule diameter is reduced. In general, there is a compromise to be found between the HTF flow rate and the capsule diameter to improve heat transfer and minimize pumping power. Khattari et al. [42] demonstrated that for reasonably low values of HTF flow rate, the use of large size of spherical capsules can be advantageous for both thermal efficiency of the packed bed and pumping performance.



Fig.7: PCM temperature variation inside the capsule for various diameter

Fig.8 illustrates the impact of tank height on the discharge duration. We notice that the higher the height of the tank, the longer the discharge period, which appears to be coherent since an increase in height, induces an increase in the number of capsules, which implies to have an important quantity of PCM to melt inside the tank.



Fig.8: HTF temperature at the tank outlet versus time for various tank size

Fig.9 shows the evolution of the HTF temperature at the tank outlet for three initial temperatures ($T_i = -8^{\circ}C$; $-6^{\circ}C$; $-4^{\circ}C$). The curves follow a completely similar pattern during the discharge. They differ only in the discharge time, which is slightly delayed as the initial temperature is raised. Therefore, the initial temperature does not have a great influence on the duration of the discharge process.



Fig.9: HTF temperature at the tank outlet versus time for various initial temperature

Conclusion

The physical model based on the apparent heat capacity method was implemented in this study. This model allowed us to analyse the phase transition inside the spherical capsules and to investigate the influence of different parameters on the thermal behaviour of the tank during the discharge period. It was also observed that the higher the height of the tank, the longer the discharge period. Increasing the diameter of capsules from 47 mm to 77 mm leads to increase the discharging period by about 30 %. In addition, varying the storage tank initial temperature between -8 °C to – 4 °C does not have a significant effect of on the discharging time.

From this investigation, we can conclude that:

• The system operation is strongly influenced by the size of the tank and the HTF flow rate.

- The reduction in capsule diameter reduces the discharge time. There is a compromise to be found between the HTF flow rate and the capsule diameter to improve heat transfer and minimize pumping power.
- The thermal performance of the system is slightly impacted by the initial conditions.

It is therefore important to dimension the storage tank according to the available power so that the discharge process is complete. The HTF flow rate will be chosen in order to recover the thermal energy stored within the required time.

Acknowledgments: This research was carried under the framework of E2S UPPA supported by the "Investissements d'Avenir" French programme managed by ANR (ANR-16-IDEX-0002)

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