

Numerical simulation of a PCM packed bed system: A review

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Abstract

The detailed study of latent packed bed thermal energy storage (TES) system has been a great topic of interest in the literature. Experimental measurements have been conducted to analyze the performance of these systems, however, the complex transient nature of latent TES makes necessary the use of numerical models for detailed study and evaluation of key design parameters, which lead to a numerous scientific contributions in the field. Different and diverse numerical models have been developed, which can be mainly divided into single phase models, Schumman's model, concentric dispersion model, and continuous solid phase model. This paper provides an extensive comprehensive revision of the different numerical models, highlighting the key aspects of each one as well as the main findings in the field. Furthermore, the performance of the different methodologies are discussed and compared. The most important empirical correlations used in the different models in order to take into account physics, such as natural convection inside the spheres or effective thermal conductivity of heat transfer fluid, are also given.

Key words

Review, Packed bed, Phase change materials (PCM), Thermal energy storage (TES), Numerical modeling

1. Introduction

Renewable energy sources play an important role in providing energy services in a sustainable manner and even though their share of global energy consumption is still small, the use of renewable energy has been increasing rapidly in recent years [1]. Moreover, according to the ETP 2012 [2], stronger energy government policy actions can help these technologies to overcome their economic and technical barriers and be widely used. One of the principal barriers stands on the intermittent nature of some

renewable sources, such as wind or solar energy, which suppose a mismatch between the energy production and demand periods.

Thermal energy storage (TES) is identified as a technology which can help in the management and control of these systems by eliminating this mismatch or by making peak load shifting strategies [3,4]. Latent thermal energy storage systems are considered to be more energy dense, efficient and compact and have been extensively studied [5-7]. Within this context, packed bed latent heat storage systems have been a great topic of interest because of the high heat transfer area between the storage (spheres of phase change material) and the heat transfer fluid (HTF).

These packed bed TES systems have been used for several applications such as, solar thermal energy storage [8], compressed air energy storage [9], solar cooling [10], CPS plants [11], low temperature storage systems for central air conditioning [12], energy efficient buildings and waste heat recovery systems [13]. The optimization of the design and control of such TES systems are mandatory to overcome the technological and economic barriers of this technology. Within this context, numerous experimental investigations have been carried out to study the thermal characteristics of the system during freezing and melting processes. Cho and Choi [14] drove a parametric study based on Reynolds number and inlet temperature to study the performance of paraffin in a packed bed system in comparison to a system with water as storage material, they concluded that the average heat transfer coefficient for paraffin were larger by a maximum of 40% than the one with water during both freezing and melting; moreover, they experimentally demonstrated that the melting process is affected by the natural convection occurring at the liquid fraction inside the PCM spheres. Nallusamy et al. [15] also used paraffin in a packed bed system to study the effect of porosity and HTF flow rate in the performance of the system, the authors conclude that the used packed bed phase change materials (PCM) reduces the size of the storage tank in comparison to conventional sensible storage tanks. Stratification inside the tank has been also experimentally investigated by Oró et al. [16] demonstrating that the use of latent heat storage packed bed increases the stratification during the discharge process.

In spite of the experimental works, the complex transient nature of the latent packed bed TES system and the high cost of the set ups, makes necessary the use of numerical

models to deeply study the performance of this system. Several different models have been developed for predicting numerically the thermal performance of a packed bed Latent Thermal Energy Storage (LTES) system (Figure 1) based on a cylindrical tank filled with spheres containing PCM.

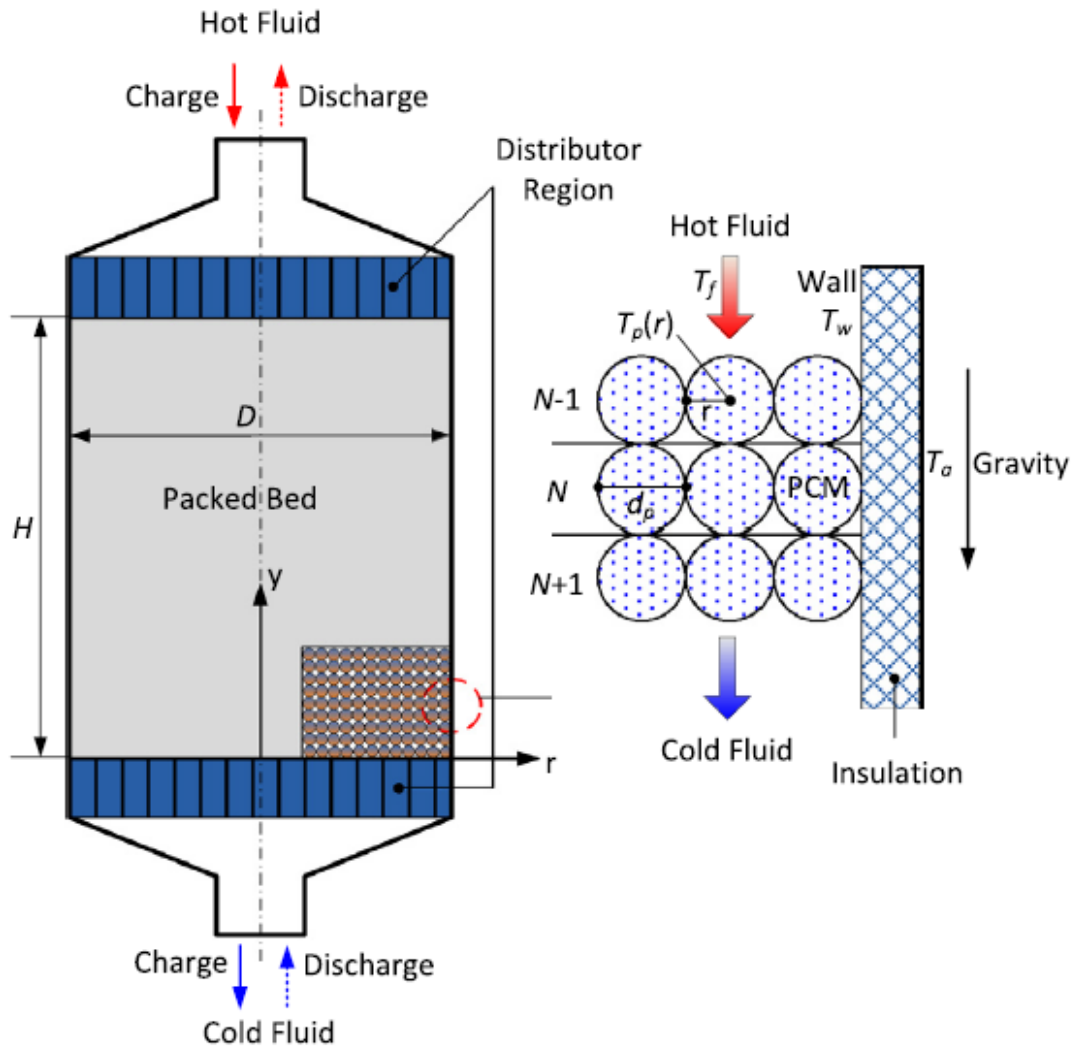


Figure 1. Sketch of a packed bed thermal storage system [17]

The objective of this paper is to provide a summary of the different numerical methodologies and empirical correlations that have been used to study these systems and present their performance and major achievements. This state of the art will be helpful for using already existing methodologies or for developing new numerical methodologies based on a combination of the previously described models.

2. General overview of the models

As it was previously stated, different numerical methods describing the performance of a latent packed bed TES systems are available in the literature [18,19]. These numerical models can be mainly divided into two groups [20]: single phase models and two phase models.

In the first group, the single phase models, the solid (PCM spheres in this case study) and the fluid phase are considered as a unique phase, considering that the instantaneous temperature of both solid and fluid phases is the same. According to Ismail and Stuginsky [21] this model is useful in analyzing fixed beds of both high thermal conductivity and thermal capacity in comparison to the working fluid. In this case, the instantaneous temperatures of the solid and fluid phases are equal.

Regarding the two phase models, solid and fluid phases are treated separately and the boundary between the solid-fluid interface is described by using Nusselt correlations. Three different typologies exist: the concentric dispersion model [10], the continuous solid phase model [22], and the Schumann's model [23]. In the concentric dispersion model the thermal conduction inside the solid is taken into account, and two different energy equations are solved altogether, one for the solid phase and one for the fluid phase. It assumes a thermal gradient inside the solid particles and no inter-particle heat transfer; hence heat is only transferred between the fluid and the bed.

On the other hand, the continuous solid phase model considers the system as a continuous porous medium and not as a medium composed of independent solids. It can include heat conduction in the axial and radial direction of both solid and fluid phases, however, it is usually discretized in one-dimension so only axial thermal conduction is considered. Using this last method it is possible to model the variation of the porosity with the radial distance and hence determine the radial distribution of the fluid velocity using the extended Brinkman equation.

Finally, the Schumann's model is a two phase model in which heat conduction is not considered neither for the axial nor the radial direction. Hence, only convection between solid-fluid phases and heat losses to the environment are integrated in the model.

All four models assume fluid flow among the solid as a kind of flow in the porous material, where the variation in the cross-sectional area of flow passages cannot be accurately reflected and an average flow rate of the fluid along the flow passages is used. In addition, the accuracy of these models depends on the effective thermal conductivity of the porous material and the total heat transfer coefficient between the fluid and the solid which are usually determined from empirical correlations.

This paper will focus on the already presented four main numerical methodologies, however, apart from these models some specific studies have been conducted using different morphologies of numerical methods. Xia et al. [20] developed a different model, called effective packed bed model, which can investigate the flow field as the fluid flows through the voids among the solids and can also account for the thermal gradients inside the PCM spheres, however, it uses a 2-D CFD model which requires an important computational effort. The model was validated against experimental data [24, 25]. A different approach was investigated by Amin et al. [26,27], here the authors used the effectiveness-NTU method to characterize a PCM packed bed system and created a correlation which provides the effectiveness of the heat transfer and the mass flow rate which can be used to predict the average thermal capacity of the system for a given flow rate.

3. Single phase models

Single phase models treated the fluid and solid phases as a unique element, hence both phases discretized altogether. Energy equation can be written as follows:

$$\varepsilon \cdot C_{p,f} \cdot \rho_{HTF} \cdot \frac{\partial T}{\partial t} + (1-\varepsilon) \rho_{PCM} \frac{\partial H}{\partial t} + C_{p,f} \cdot \rho_f \cdot u \cdot \frac{\partial T}{\partial y} = k_{eff,y} \frac{\partial^2 T}{\partial y^2} + k_{eff,r} \left(\frac{\partial^2 T}{\partial r^2} + \frac{\partial T}{2 \partial r} \right) \quad (\text{Eq.1})$$

The first two terms of the expression stands for the accumulative term of the heat transfer fluid and the PCM, respectively. The last term in the left-hand reflects the convective term of the HTF, the two terms in the right-hand side reflect the conduction in the axial and radial direction, respectively. Heat losses to the environment can be added in the boundary nodes.

The use of this methodology is not popular when describing PCM packed bed systems because the assumption that the HTF and PCM are at the same instantaneous temperature in only valid when using solid particles with very high thermal

conductivity. The limited thermal conductivity in the PCM is well known, being around 0.2 W/m·K in paraffin and fatty acids and around 0.6 W/m·K in salts hydrate [7, 28].

However, Nagano et al. [29] proposed a single phase model to study the performance of an air direct heat exchanger with PCM granules. The small dimension of the particles justifies the use of this model. An experimental set-up was design to validate the model with temperature sensor at different heights inside the tank. The model considered one-dimensional flow, and even air and PCM are considered to have the same temperature at each location, only the PCM accumulative term is considered. The energy conservation equation was solved using an explicit finite difference method. The authors demonstrated with the experimental and numerical results that the amount of heat per unit time and unit area can be large during phase change in the system.

4. Schumann's model

This two phase model assumes one dimensional heat transfer and does not consider heat conduction neither in the fluid nor in the solid phases. As in all the two phase models, the energy conservation equations are written separately for the HTF (Eq.2) and the solid particles (Eq.3) and have to be solved simultaneously.

$$\varepsilon \cdot C_{P,f} \cdot \rho_f \left(\frac{\partial T_f}{\partial t} + u \frac{\partial T_f}{\partial y} \right) = h_{PCM-HTF} (T_{PCM} - T_f) - U_L (T_f - T_{ENV}) \quad (\text{Eq.2})$$

$$(1 - \varepsilon) \rho_{PCM} \frac{\partial H}{\partial t} = h_{PCM-HTF} (T_f - T_{PCM}) \quad (\text{Eq.3})$$

This methodology was one of the first attempts to describe numerically the behavior of packed bed thermal storage systems. Its simplicity stands in taking a lumped capacitance approach to the solid particles and assuming the convection coefficients independent of time and space. Sanderson and Cunningham [30] used this simple model to investigate how the particle diameter affects the degree of axial dispersion as well as the pressure drop.

The principal limitation of the Schumann's model is that it cannot take into account thermal diffusion inside the solid particles, hence no thermal gradients are considered in the spheres and heat conduction is not considered in the model as only convection is

driving the heat transfer process. However, as it was previously stated, the PCM are characterized by their low thermal conductivity, which makes heat conduction thermal resistance to play an important role in the heat transfer during both charge or discharge processes. Therefore, some authors have adapted the Schumann's model in order to take into account the conductive thermal resistance by adding into the convective heat transfer at the solid-fluid boundary the conductive thermal resistance of the sphere.

Regin et al. [31, 32] adapted the Schumann's model to study the behavior of a packed bed latent heat thermal energy storage used for a solar water heating system. The model includes the conductive resistive layers of the shell and solid parts of PCM into the energy equation at solid-fluid boundary by using an outer surface overall heat transfer coefficient U_0 . This coefficient varies depending on the phase of the spheres: fully liquid, fully solid or during phase change. And it is defined as follows:

$$U_0 = \frac{1}{A \cdot R_{ext} + R_c + R_{in}(t)} \quad (\text{Eq.4})$$

where R_{ext} is the convective thermal resistance, R_c is the thermal resistance due to conduction of the capsule shell and $R_{in}(t)$ is the resistance due to the solidified/melt PCM layer inside the capsule, which is function of time, as shown in Figure 2. Hence, even the model do not discretize the spheres, it takes into account the conduction inside by modifying the heat transfer coefficient between PCM and the heat transfer fluid.

The phase change is taken into account using the enthalpy method and even the model does not present any validation against experimental data, the authors conclude that the required period for a full solidification is much longer than the one required for a full melting of the PCM and that the charging and discharging rates are much higher if reducing the diameter of the capsules.

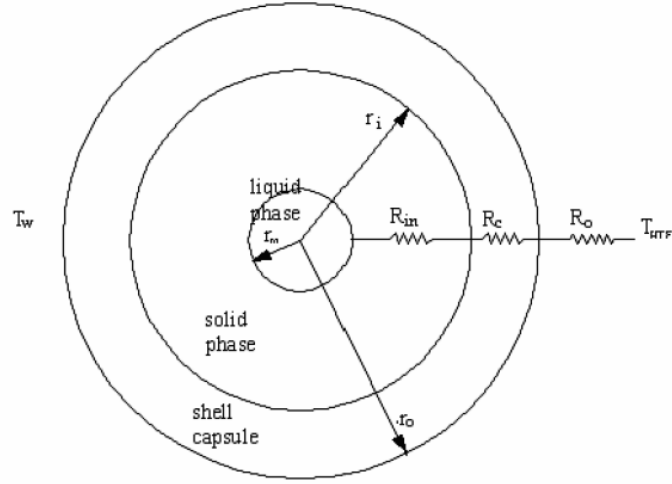


Figure 2 . Sketch of the thermal resistances considered in the model [32]

A similar adaption of the Schumann's model was used by Tumilowicz et al. [33] to study the performance of a thermocline with PCM packed bed storage. Here the authors used an effective convective heat transfer in the case that the size of encapsulated filler is large and gives a large Biot number [34, 35]. The authors used the method of characteristics to solve the system of algebraic equations. The results were verified against analytical solutions and demonstrated that the operation of thermocline can be predicted without consuming high computational resources using the method of characteristics.

5. Concentric dispersion model

This method is based on a two-phase model and treats the packed bed as an isotropic porous medium consisting of independent spherical particles. This approach is the only that solves the thermal distribution inside the solid particles. It can include axial heat conduction in the heat transfer fluid and/or in the PCM. Hence the energy conservation equation can be written as Eq.5 (HTF), Eq.6 and Eq.7 (PCM at boundary and PCM inside the sphere, respectively).

$$\varepsilon \cdot C_{p,f} \cdot \rho_f \left(\frac{\partial T_f}{\partial t} + u \frac{\partial T_f}{\partial y} \right) = \varepsilon \cdot k_f \frac{\partial^2 T}{\partial y^2} + h_{PCM-HTF} (T_{PCM} - T_f) - U_L (T_f - T_{ENV}) \quad (\text{Eq.5})$$

$$(1 - \varepsilon) \rho_{PCM} \frac{\partial H}{\partial t} = (1 - \varepsilon) k_{PCM} \frac{\partial^2 T}{\partial y^2} + h_{PCM-HTF} (T_f - T_{PCM}) \quad (\text{Eq.6})$$

$$\rho_{PCM} \frac{\partial H}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left(k_{PCM} \cdot r^2 \cdot \frac{\partial T}{\partial r} \right) \quad (\text{Eq.7})$$

In the concentric dispersion models the cylindrical container is divided into elements in the axial direction in which fluid temperature is considered uniform. All the spheres at the same height are considered to behave equal, moreover, usually only one sphere is discretized and solved as shown in Figure 3. Moreover, it is very simple to implement heat losses to the environment in such models.

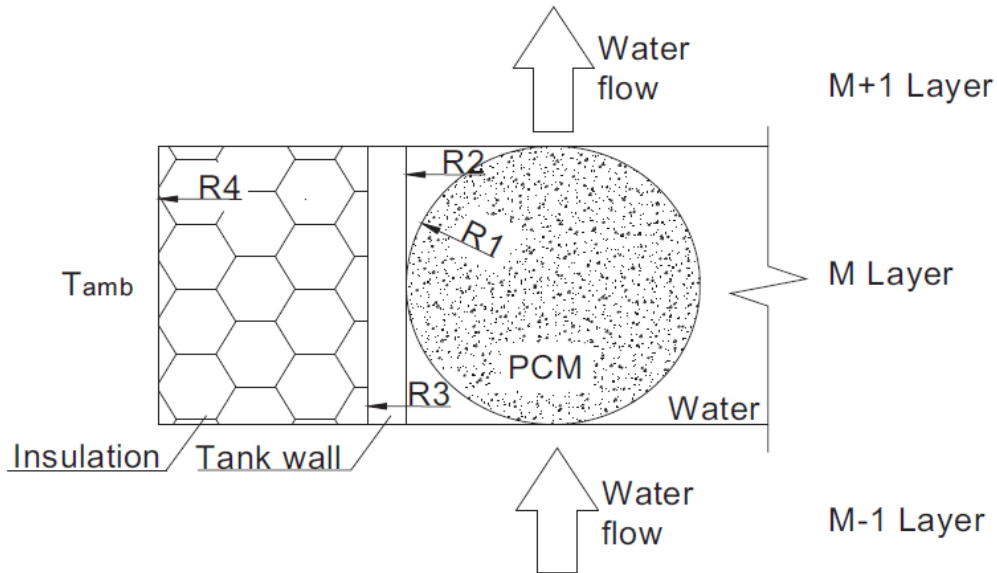


Figure 3 . Sketch of discretized domain in Concentric Dispersion Method [36]

A concentric dispersion model was developed by Ismail and Henríquez [37], where the tank is divided into a number of axial layers and the fluid only exchanges heat with the particles. Moreover, the model takes into account the natural convection of the liquid phase of the PCM using an effective thermal conductivity. The model was validated using experimental data provided by the authors and is solved using a finite difference approach and moving grid technique. The working fluid entry temperature, the mass flow as well as the capsule temperature were investigated.

In the same way, Wu et al. [38] used a similar approach but with considering axial heat conduction in for the bed and the fluid. The model also uses an effective thermal conductivity to predict natural convection inside the PCM particles. However, the heat losses to the environment are not considered and the phase change is considered to occur at a unique temperature, the model was not validated against experimental data. The study concludes that the latent heat storage capacity of the PCM spheres is only about 70% of the total heat storage capacity of the system, which is due to the sensible cooling of the PCM and HTF.

Another concentric dispersion model was developed by Bédécarrats et al. [39]. Here, in order to determine the heat transfer coefficient between the solid spheres and the HTF, the ratio between Gr/Re^2 is used. In the case that this ratio is higher than the unit, free convection is considered dominant in comparison to forced convection. The numerical model was validated against experimental data [40] and was used to study the effect of the final inlet temperature and the inlet flow rate on the time for complete storage. Moreover, Galione et al. [41] incorporated the momentum equation in the heat transfer fluid to study the performance of a thermocline-PCM thermal storage concept for CSP plants. The model was validated against the experimental data from Pacheco et al. [42] and conclude that the PCM layers if located at the top and bottom of the thermocline act as a thermal buffers, forcing the outlet temperature of the tank be close to the fusion temperatures and hence inside the desired thermal range of the application. Furthermore, Galione et al. [43] demonstrated that the use of multilayered solid-PCM prevents thermocline degradation, increasing the efficiency in the use of the overall thermal capacity of the system, and requires less amount of encapsulated PCM than a cascaded PCM concept to store almost the same energy. The same system was analyzed economically by Zhao et al. [44] concluding that multi-layered solid-PCM thermocline concept with an optimum configuration is more cost-competitive than any other thermocline TES system on the same design requirements and operating conditions.

Yang et al. [45] modeled a storage packed bed tank with PCM having different melting points. The model, based on concentric dispersion method, presents one dimensional assumptions and includes the natural convection inside the spheres by using an effective thermal conductivity. Moreover, heat conduction of the HTF in the axial direction is considered using another correlation that modifies the thermal conductivity of the HTF. The numerical solution was based on control volume integration method using a fully implicit time integration scheme. The results were validated against experimental measurements [25] and are used to demonstrate that the system with PCM multiple-type packed bed melts faster than the single-type one. It was also highlighted that during the melting process the multiple-type presents higher energy transfer efficiency.

A similar model was developed by Ereik and Dincer [46] to test a newly developed correlation to determine the heat transfer coefficient between the PCM particles and the

HTF. The authors claimed that in the correlations of the literature, the heat transfer coefficient is considered constant as the flow is assumed hydrodynamically and thermally developed. However, experimental results indicated that the coefficient varies greatly during downstream and highly affects the heat transfer taking place during the process. A set of CFD simulations was carried out to perform the new Nusselt correlation, which was validated against experimental data from Eames and Adref [47].

Molten salts are used as a HTF in the packed bed latent heat thermal energy storage system analyzed by Peng et al. [17]. The authors developed a numerical model based on the concentric dispersion methodology and use non-dimensional parameters to solve and generalize the model and the corresponding results. A mesh independent study was carried out to prove that the numerical model is consistent with 2500 elements. The numerical model is validated against experimental data from Izquierdo-Barrientos et al. [48] with average deviations of 5%. The study concludes that the particle size is a dominant parameter in the heat transfer between the HTF and the PCM. Smaller the particle diameter, the HTF temperature starts to increase later and the effective charge time is shortened, thus increases the charge efficiency. It was also demonstrated that the increase of the inlet velocity results in a decrease of charge efficiency, as well as, the use of higher thermal storage tank provides higher charge efficiency.

Furthermore, Bindra et al. [49] carried out an exergy calculation for packed bed using an experimentally validated numerical model which takes into account heat losses to the environment, thermal gradient inside the spheres and axial heat transfer in the HTF and the PCM. The parametric study carried out in the paper showed that in the case of high storage temperatures, in order to obtain higher exergy recovery with PCM storage systems, these should have lower latent heat or lower energy density, since in the case of sensible heat storage system even at high energy density, higher exergy recovery can be obtained. PCM is particularly useful if the heat is needed at a temperature near the phase change.

Karthikeyan et al. [50] used a concentric dispersion model to describe a solar system with air as HTF. The model used the enthalpy method to model the phase change. In this paper different parameters were studied in order to increase the heat transfer rate in both charging and discharging processes. It was demonstrated that in this case study the

thermal conductivity of the PCM is not as critical as the low convective term because of the use of air as HTF. However, the model was used to demonstrate and quantify the effect of the PCM sphere size, the inlet HTF temperature and the effect of the mass flow rate of the HTF.

Concentric dispersion model has been also used to test the dynamic behaviour for charging/discharging processes of the molten salt packed bed TES system filled with high-temperature PCM capsules. Wu et al. [51] compared numerically the performance of non-cascaded against 3 and 5 cascaded phase change temperature systems, showing that the non-cascaded suffer from the low charging ratio requiring long charging time.

Finally, Kousksou and Bruel [52] used this methodology to test a packed bed storage system when various complex input temperature signals are considered. The system is altered significantly when some randomness is introduced at the inlet, explaining why in some cases, the PCM systems in real applications do not prove the same performance as priori expected.

6. Continuous solid phase model

The continuous solid phase model considers the system as a continuous medium and not as a medium comprised of individual particles. Hence, even thermal gradients inside the particles cannot be modeled, the heat conduction in the packed bed can occur in the axial direction (one dimensional continuous solid phase models) or in axial and radial direction (two-dimensional continuous solid phase models). Even though the addition of heat transfer in the radial direction increases strongly the computational cost of the model, is the only model able to capture thermal gradients in this direction, which may gain importance in system with low mass flow rates subjected to heat losses to the environment or to system with inlet flows not well distributed. Since this methodology is a two phase model, fluid (Eq.8) and solid (Eq.9) energy equations are written separately and solved altogether.

$$\varepsilon \cdot C_{p,f} \cdot \rho_{HTF} \left(\frac{\partial T_f}{\partial t} + u \frac{\partial T_f}{\partial y} \right) = k_{f,y} \frac{\partial^2 T_f}{\partial y^2} + k_{f,r} \left(\frac{\partial^2 T_f}{\partial r^2} + \frac{1}{r} \frac{\partial T_f}{\partial r} \right) + h_{PCM-HTF} (T_{PCM} - T_f) - U_L (T_f - T_{ENV}) \quad (\text{Eq.8})$$

$$(1-\varepsilon)\rho_{PCM}\frac{\partial H}{\partial t}=k_{PCM,y}\frac{\partial^2 T_{PCM}}{\partial y^2}+k_{PCM,r}\left(\frac{\partial^2 T_{PCM}}{\partial y^2}+\frac{1}{r}\frac{\partial T_{PCM}}{\partial r}\right)+h_{PCM-HTF}(T_f-T_{PCM}) \quad (\text{Eq.9})$$

Cheralathan et al. [53] developed and validated experimentally a one-dimensional continuous solid phase model to carry out a parametric study on the performance of a cool thermal energy storage system. The model assumes that the HTF is fully developed and the storage tank is well insulated. The thermal conductivity of the fluid and the particles are used directly, without using correlation for effective thermal conductivities. The authors design and test an experimental set-up to validate the model. The authors studied the influence of porosity, Stephan and Stanton numbers. Similarly, Hu et al. [54][54] also developed an experimental set-up to validate a similar model used to optimize the design of a direct contact condenser used in a solar driven humidification-dehumidification desalination plant. Here, two-phase HTF (air and water) is considered in the model. The analysis concluded that for this application a water to air mass flow ratio around 1.5 is advised, and that the use of small high thermal conductivity particles are the ideal candidates instead of PCM.

Another one-dimensional continuous phase model was developed by Aldoss and Rahman [55] to compare the performance of a single-PCM and multi-PCM packed bed thermal energy storage systems. The authors demonstrated that using multi-PCM design provides higher performance in both charging and discharging processes. However, using more than three stages of PCM inside the packed bed do not provide significant improvements. Multiple layer packed bed system was also studied by Zanganeh et al. [56] using a one dimensional continuous phase model. In that case, instead of multiple layers of PCM the authors proposed a novel thermal energy storage for concentrated solar thermal power based on a packed bed of rocks with a small amount of PCM at the top of the bed. The addition of the PCM stabilizes strongly the outflow temperature during discharging, eliminating temperature drop from sensible heat storage systems. Even the model does not consider thermal gradients inside the spheres, the convection heat transfer coefficient was adjusted to consider the intra-particle conduction [57].

Similarly Wu and Fang [58] used an effective convective heat transfer coefficient in a one-dimensional phase model, where the conductive thermal resistance of the spherical shell and PCM is included in the convective term that describes the solid-fluid

boundary. The authors studied the performance of a packed bed system when using myristic acid as phase change material. This model does not include natural convection of the PCM spheres, however, it considered heat losses through the tank wall. The numerical results were compared against experimental data from Nallusamy et al. [25]. In addition, the same model was used by Wu et al. [59] to evaluate the performance of n-tetradecane as PCM in a packed bed cool thermal energy storage system. In the model used in both studies, the thermal conductivity of the HTF is assumed directly to drive the conduction inside the continuous media. However, Ismail and Stuginsky [21], highlights the importance of using an effective thermal conductivity in order to consider in the model conduction through the solid particles, conduction through the contact solid, radiation between the solid surfaces, film convection through the fluid layer involving the solid particles, and others.

In this way Rady [60] used an effective thermal conductivity in the axial direction. Here, an important innovation was provided since the model was able to evaluate the performance of multiple granular phase change components. The author distinguished the latent heat and their melted fraction of the two different materials. After an experimental validation process, the model was used into a parametric study to study the mixing ratio and Reynolds number for constant inlet charging and discharging temperatures. It was concluded that an appropriate selection of the mixing ratio will lead to a significant enhancement of the overall storage unit performance in comparison to the single granular phase change material composite. This optimum mixing ratio is independent of the value of Reynolds number. Moreover, an exergy analysis was conducted to demonstrate that the use of these systems reduces significantly the exergy destroyed.

Benmansour et al. [61] used effective thermal conductivity for the fluid both for axial and radial heat transfer. They developed a two-dimensional continuous solid phase model using air as HTF. The fluid energy equation was transformed using finite differences and solved implicitly while the solid particles was solved using fully explicit scheme. Arkar et al. [62] also uses two dimensional continuous solid phase model to study the performance of a free cooling system based on two packed bed latent heat thermal energy storage systems. The authors justified considered an adaptation of the mathematical model because a non-uniform radial distribution of the axial fluid velocity

due to small tube-to-sphere diameter ratio. The numerical model was used to predict the heat storage outlet air temperature and create Fourier series which were implemented into TRNSYS simulation program.

7. Model comparison studies

Ismail and Stuginsky [21] compared the performance of the main four models for the same case study and evaluated the computational resources required in each case. Using the same computer SPARC stations1 +, with FPU Weitec 3170-25 MHz it provides the results presented in Table 1. The results highlights the increment in the computational time due to the use of two-dimensional approach instead of considering just one-dimensional conditions, being around 20 times longer in both cases single phase models and continuous solid phase models. Therefore, the addition of heat transfer in the radial direction of the packed bed is just recommended if well justified for detailed case studies with non-uniform inlet distribution or cases with low mass flow rates and important heat losses to the environment.

Table 1. Computational cost of each model [21]

Model	CPU Time (s)
Single phase model 1D	7.1
Single phase model 2D	141.5
Schumann's model	29.6
Continuous solid phase model 1D	51.6
Continuous solid phase model 2D	1277.7
Concentric dispersion model	574.6

Karthikeyan and Velraj [63] compared against experimental data the performance of three different numerical models. The first is a Schumman's model in which all the PCMs at a particular height of the tank are considered to be at the same temperature at a particular time and conduction along the axial and radial direction is neglected. The second is a continuous solid phase model in which conduction effect along the axial direction of HTF and PCM is included but not the radial. Finally, the third is a concentric dispersion model hence thermal gradients inside the capsules can be simulated. The validation procedure shows that only the third method is able to predict

accurately the performance of the system. This is justified because the low thermal conductivity of the PCM affects drastically in the internal conductive resistance of the spheres. Moreover, non-significant differences were found between the Schumman's model and the one-dimensional continuous solid phase model.

Moreover, Galione et al. [64] developed a concentric dispersion model and compared its performance against a 2D CFD model. In the one-dimensional model the domain is discretized and the mesh independent study was achieved at $N_x=24$ (nodes at the vertical axis) an $N_r=12$ (radial nodes inside the sphere). The model used a finite volume approach to solve the fluid and solid energy balances. On the other hand the CFD model was validated against experimental data [65, 66] and can predict the natural convection because of difference of density and gravity action, inside the sphere in the liquid phase. However, the authors concluded that similar numerical results were obtained using the simplified 1D method and the CFD. Moreover, when using the CFD tool, the system needed 4 days to simulate 5 hours of operation using a 48 CPU cores in parallel (AMD Opteron Barcelona 2.1 GHz, Infiniband network 4X-DDR 20 Gb/s).

Oró et al. [36] also compares the performance of two different numerical approaches. In this case, a continuous model based on Brinkmann equation and a second model based on concentric dispersion methodology. The Brinkman's equation is a transition from the Darcy model (which assumes that all the stress in the flow field is carried by the porous medium and the fluid is not subjected to any strain because of the viscous stress), to viscous free flow, since it has been demonstrated that Darcy model cannot be used alone because in high permeability porous media, at least part of the viscous stress became from the fluid itself [67]. The first model can simulate the gravitational forces inside the flow but it cannot take into account the thermal gradient inside the PCM spheres. The comparison against experimental data show good agreement with the two models, and it was demonstrated that the free convection is not as important as forced convection in the studied case.

8. Empirical correlations

As it has been previously discussed in the paper, in order to save computational cost, different physics are introduced in the numerical models by using empirical correlations

from the literature. In this chapter, the different empirical correlations used for modeling latent packed bed systems will be given.

8.1 Nusselt correlation for fluid-solid interface

These set of empirical correlations are used to define the convective heat transfer occurring between the solid particles and the heat transfer fluid. They are used in all the two phase models: Schumann's model, concentric dispersion model and continuous solid phase model.

One of the most used empirical correlations is the one provided by Beek [68], which is given in Eq.10, which determines the Nusselt number in the case of capsules arranged in a random form.

$$Nu = 3.22 \cdot Re^{1/3} Pr^{1/3} + 0.117 \cdot Re^{0.8} Pr^{0.4} \quad (\text{Eq.10})$$

The correlation of Wakao and Funazkri [69] gives the Nusselt number in forced convection conditions and is valid when $15 < Re < 8500$. The correlation presented in Eq.11 has been used in concentric dispersion models [31, 64] and continuous solid phase models [55], and is the only one altogether with the one proposed by Perry and Green [70] (Eq.12), in which Nusselt number is function of the porosity of the packed bed.

$$Nu = 2 + 1.1 \cdot [6 \cdot (1 - \varepsilon)]^{0.6} Re^{0.6} Pr^{1/3} \quad (\text{Eq.11})$$

$$Nu = 3.6 \left(\frac{d_p G}{\mu_f \cdot \varepsilon} \right)^{0.365} \quad (\text{Eq.12})$$

Moreover Galloway and Sage [71], proposed another Nusselt correlation (Eq.13) which was used in Benmansour et al. [61]:

$$Nu = 2 + 2.03 \cdot Re^{0.5} \cdot Pr^{0.33} + 0.049 Re Pr^{0.5} \quad (\text{Eq.13})$$

In the cases with very low Reynolds number ($Re < 40$), the correlation of Vafai and Sozen [72] given in Eq.14 is proposed.

$$Nu = 18.1 \cdot Pr^{1/3} \quad (\text{Eq.14})$$

In addition, Bédécarrats et al. [39] used the ratio of Gr/Re^2 to determine the weight of the natural convection in comparison to forced convection. If the ratio is similar or

lower than the unit, a forced convection correlation is proposed (Eq.15), on the other hand, if natural convection is dominant the correlation from Churchill [73] is applied (Eq. 16).

$$Nu = Re^{0.5} \cdot Pr^{0.33} \quad (\text{Eq.15})$$

$$Nu = 2 + \frac{0.589 \cdot Ra^{0.25}}{\left[1 + \left(\frac{0.469}{Pr}\right)^{9/16}\right]^{4/9}} \quad (\text{Eq.16})$$

8.2 Axial effective thermal conductivity

The heat transfer occurring in the HTF and in the axial direction is considered in most of the continuous solid phase models and in some of the concentric dispersion models. Instead of using directly the thermal conductivity of the fluid, the authors used empirical correlations to determine an effective thermal conductivity. In this way, Yang et al. [45] proposed the correlation given in Eq.17.

$$k_{eff,y} = 0.5 \cdot Re \cdot Pr \cdot k_f \quad (\text{Eq.17})$$

Similarly, Wu et al. [38] used the previous correlation, however, in cases with low Reynolds number ($Re < 0.8$), the effective thermal conductivity does not depend on Prandtl number (Eq. 18) and so it does on porosity.

$$k_{f,y} = 0.7 \cdot \varepsilon \cdot k_f \quad (\text{Eq.18})$$

Furthermore, Rady [60] stated that the effective thermal conductivity consists of the stagnant and the dispersion conductivity. The dispersive component in the longitudinal thermal conductivity in the porous media was evaluated using the correlations based on the Peclet number [74, 75] (Eq.19 and Eq.20) .

$$k_{eff,y} = k_f + 0.022 \cdot k_f \frac{Pe^2}{1 - \varepsilon} \quad \text{for } Pe < 10 \quad (\text{Eq.19})$$

$$k_{eff,y} = k_f + 2.7 \cdot k_f \frac{Pe^2}{\varepsilon^{0.5}} \quad \text{for } Pe < 10 \quad (\text{Eq.20})$$

8.3 Effective thermal conductivity of PCM due to natural convection

The low thermal conductivity of the PCM affects drastically the charge and discharge processes occurring in packed bed systems. However, during the charge process, natural

convection inside the PCM spheres enhances significantly the heat transfer rate. The authors of some concentric dispersion models have considered this physics by using an effective thermal conductivity inside the spheres, which is function of Rayleigh number. This effective thermal conductivity is just applied to the liquid region of the spheres and its value varies during the process as it does Rayleigh number. The most used correlation is the one proposed by Chiu and Chen [76], given Eq.21.

$$k_{eff} = 0.18 \cdot k_s \cdot Ra^{0.25} \quad (\text{Eq.21})$$

Moreover, the correlation of Raithby and Hollands [77] is also presented, in which a coefficient for spherical geometries, F_{sph} , is used (Eq.22).

$$k_{eff} = 0.74 \cdot k_s \cdot [\text{Pr}/(0.861 + \text{Pr})]^{0.25} \cdot (F_{sph} \cdot Ra)^{0.25} \quad (\text{Eq.22})$$

8.4 Other correlations

The value of the void fraction is usually determined by the authors as a constant, however, some authors determined this value according to the correlation proposed by Beavers et al. [78], which is function of the diameter of the tank and the spheres diameter (Eq.23):

$$\varepsilon = 0.4272 - 4516 \cdot 10^{-3} (D/d_p) + 7.881 \cdot 10^{-5} (D/d_p)^2 \quad (\text{Eq.23})$$

Apart from the previously detailed empirical correlations, the authors have used others for describing different physics, such as heat losses to the environment or pressure drop.

The heat losses to the environment are calculated by using a volumetric coefficient which is based on an internal convective resistance, conductive resistances and an outer convective resistance. According to Kreith et al. [79], the internal one is calculated using the Nusselt correlation from Eq.24.

$$Nu_{in} = 2.58 \cdot \text{Re}^{1/3} \text{Pr}^{1/3} + 0.094 \cdot \text{Re}^{0.8} \cdot \text{Pr}^{0.4} \quad (\text{Eq.24})$$

Moreover, the Nusselt correlation to determine the outer convective heat transfer coefficient is proposed by VDI Gesellschaft [80] (Eq.25).

$$Nu_{out} = \left[0.825 + 0.387 \left[Ra \left[1 + \left(\frac{0.492}{Pr} \right)^{\frac{9}{16}} \right]^{\frac{-16}{9}} \right]^{\frac{1}{6}} \right]^2 \quad (\text{Eq.25})$$

Finally, some authors calculated the pressure drop across the thermal storage packed bed system using the correlation given in Eq.26 [81, 82] :

$$\Delta P = 150 \cdot L \frac{1 - \varepsilon}{\varepsilon^2} \frac{\mu_f \cdot u}{d_p^2} + 1.75 \cdot L (1 - \varepsilon) \varepsilon \cdot \frac{\rho_f \cdot u^2}{d_p} \quad (\text{Eq.26})$$

9. Conclusions

The present paper reviews and discusses the different numerical methodologies available in the literature which are used to predict the performance of latent packed bed thermal energy storage systems. In spite of the diversity of models, they can be grouped into single phase models and two phase models.

Single phase models are computationally cheap; however, they can only be used in systems in which the heat transfer fluid and particles have high thermal conductivity and thermal capacity or in systems with very small particles. From the two phase models, the Schumann's model is the simplest because it assumes infinite thermal conductivity in the particles, hence no thermal gradients can be modeled. On the other hand, concentric dispersion models require high computational cost since they solve the thermal map inside the PCM particles, including the effect of natural convection in some cases. Finally, the continuous solid phase models can discretize in one or two dimensions the packed bed. The discretization of the packed bed in the radius direction is very limited in the literature because it increases dramatically the computational time; however, it is the only way to deeply study some key aspects such as the effect of different porosity or fluid velocity at different positions in the packed bed.

The numerical studies have been used for diverse specific applications, however, some main conclusions can be highlighted:

- The amount of heat per unit time and unit area can be large during phase change in the system.
- The particle size is a dominant parameter, the use of smaller particles increases the charge efficiency.
- Around 70% of the total heat storage capacity of packed bed systems is due to the latent heat, the other is sensible of PCM and HTF.
- The use of PCM multiple-type packed bed presents higher energy transfer efficiency and power of heat exchange in comparison to single-type packed bed systems.
- The use of multiple granular phase change components can lead to an enhancement of the system performance.
- In systems in which air is the HTF, the low thermal conductivity of the PCM is not as critical as the low convective term.

All the previous mentioned methodologies used empirical correlation to determine key physical aspects such as convective heat transfer at the solid-fluid interface, natural convection inside liquid region of PCM spheres or effective thermal conductivity. The most important empirical correlations used in the literature to describe these physics are also given in the present paper.

Nomenclature

C_p	Heat capacity	$[J\ g^{-1}\ K^{-1}]$
D	Diameter of tank	$[m]$
d_p	Diameter of spheres	$[m]$
Gr	Grasshoff number	$[-]$
H	Total volumetric enthalpy	$[J\ m^{-3}]$
h	Heat transfer coefficient	$[W\ m^{-2}\ K^{-1}]$
k	Thermal conductivity	$[W\ m^{-1}\ K^{-1}]$
L	Height of the tank	$[m]$
P	Pressure	$[Pa]$
Pe	Pecklet number	$[-]$
Pr	Prandtl number	$[-]$
Re	Reynolds number	$[-]$
r	Radius direction	$[m]$
u	Velocity in y-direction	$[m\ s^{-1}]$
U	Thermal transmittance	$[W\ m^{-2}\ K^{-1}]$
t	Time	$[s]$

T	Temperature	[K]
y	Axial direction	[m]

Greek symbols

ρ	Density	[kg m ⁻³]
ε	Porosity	[-]
μ	Dynamic viscosity	[Pa·s]

Subscripts

eff	Effective
ENV	Environment
f	Fluid
HTF	Heat transfer fluid
L	Losses
p	particle
PCM	Phase change material

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