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Research Paper

Efficient simulation strategy for PCM-based cold-energy storage systems

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HIGHLIGHTS

- Computationally efficient modelling of PCM-based cold-energy storage systems.
- The efficient model is intended to be combined with that of the refrigeration cycle.
- Comparison with a precise discrete model regarding computational cost and accuracy.
- Relative errors remain below 3% while computational load is reduced by up to 99%.
- Long-term energy management strategies are to be addressed using the proposed model.

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ABSTRACT

This paper proposes a computationally efficient simulation strategy for cold thermal energy storage (TES) systems based on phase change material (PCM). Taking as a starting point the recent design of a TES system based on PCM, designed to complement a vapour-compression refrigeration plant, the new highly efficient modelling strategy is described and its performance is compared against the pre-existing one. The need for a new computationally efficient approach comes from the fact that, in the near future, such a TES model is intended to be used in combination with the model of the own mother refrigeration plant, in order to address efficient, long-term energy management strategies, where computation time will become a major issue. Comparative simulations show that the proposed computationally efficient strategy reduces the simulation time to a small fraction of the original figure (from around 1/30th till around 1/120th, depending on the particular choice of the main sampling interval), at the expense of affordable inaccuracy in terms of the PCM charge ratio.

1. Introduction

Cold-energy production via vapour-compression systems is definitively the most common method used worldwide. Significant efforts to increment energy efficiency while reducing environmental impact of current vapour-compression systems have been carried out in recent years. A novel line of research focuses not just on efficient cold-energy generation, but also on cold-energy management, including thermal energy storage systems (TES). The main idea is to use a certain reservoir to manage cold energy, in such a way that it can be stored and released according to the needs at any given time. This strategy allows to streamline the design stage, helping to avoid any undesirable oversizing of the system, in order to satisfy peak demand periods. Thereby, the equipment can be more efficiently used and energy consumption can be reduced [1,2].

From an economic point of view, TES systems enable the scheduling of cold-energy production, so that the consumer benefits from low-price time slots, typically, when global demand is lower (*peak-shifting*) [3]. Several works in the literature address management of TES systems, following different control strategies [4–6].

Regarding the design of the cold-energy reservoir, storage tanks filled with phase change material (PCM) have become a successful trend over sensible-heat materials, due to their convenient thermodynamic properties for heat transfer. Not only their heat capacity is a very relevant factor, but also the fact that their temperature does not vary significantly, provided that the material remains in latent zone, which boosts heat transfer [7]. A number of solid–liquid phase change materials designed for cold-energy storage applications can be found in the literature, including commercial and developing solutions [7–9].

Different technologies regarding latent heat TES based on PCM have been proposed and experimentally tested in the literature, where a variety of geometries and fluid arrangements can be found [8,10,11].

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Packed bed technology is among the most common configurations, where a certain volume includes a large number of small PCM nodules. First, cold heat transfer fluid (HTF) is used to charge the system by flowing through the volume and solidifying the PCM nodules. Afterwards, warm HTF circulates while melting the PCM nodules to discharge the system, which releases the previously stored cold energy [12].

Note that the same HTF is used within the packed bed technology to charge and discharge the system. However, in the application proposed in this work, the cold-energy storage tank is projected to complement an existing vapour-compression refrigeration facility. Then, the simultaneous operation of the refrigeration cycle is intended to charge the TES while satisfying the cooling demand, in such a way that the cold HTF would correspond to the refrigerant during the charging stage. Furthermore, the objective is to remove heat from a secondary fluid, so that the warm HTF would not correspond to the refrigerant, but to another secondary fluid. This key difference with respect to the standard packed bed technology implies that an original hybrid structure has to be considered, where two different HTFs are involved. Besides, the tank is filled with PCM nodules, bathed in a certain liquid, called *intermediate fluid*, while two bundles of pipes, corresponding to the refrigerant and the secondary fluid, run through the tank, being also dipped in the intermediate fluid (the constructive technical details can be found in a recent work by Bejarano et al. [13]).

Concerning modelling, much effort has been devoted to packed bed technology [14–17]. The problem of predicting the behaviour of PCM-based systems is difficult to solve, given its non-linear nature. Moreover, there are moving interfaces whose displacement is determined by the latent heat stored or released at the boundary. Therefore, the position and velocity of those boundaries are not known *a priori*.

There are two main approaches to model the behaviour of PCM-based systems. The first one relies on analytical models, using first-principle equations, whereas the second one involves numerical finite-element methods. Some relevant works of both modelling strategies are mentioned below.

On the one hand, regarding the analytical models, Bédécarrats et al. study the behaviour of a test plant, consisting of a cylindrical tank containing spherical nodules, filled with phase change material, through which a liquid fluid flows for latent heat storage purpose [18,19]. The tank is divided in several control volumes and the PCM nodules are considered as exchangers, in such a way that the transferred energy flux is proportional to the temperature difference between the fluid and the spherical nodule. The modelling of the heat flux transferred by each nodule considers a pure-conduction problem, as well as the dynamic evolution of the radius of the spherical boundary between the solid and liquid PCM phases inside the capsule. It is stated that, in the discharge, an *effective* thermal conductivity of the liquid phase must be considered to model internal convection during melting. It is concluded that the simplified model considering the nodules as exchangers confirms the experimental results with reasonable accuracy.

Alternatively, Ismail and Moraes present a quantitative study of the solidification of the PCM enclosed in a spherical shell [20]. The mathematical model is also based on pure conduction in the PCM, subject to the boundary condition of constant surface temperature. The model is validated experimentally and the agreement is found to be satisfactory.

Furthermore, Amin et al. experimentally study the freezing and melting of PCM encapsulated in a sphere [21]. They confirm empirically that the pure-conduction model is realistic when charging the PCM spheres, since the buoyancy forces have a negligible impact on the freezing process. However, as stated by other authors, it is necessary to consider an *effective* thermal conductivity of the liquid phase during the discharge to retain the spherical geometry.

Recently, Bejarano et al. have presented a continuous model of a novel TES system combined with a refrigeration cycle based on PCM, using the configuration previously described [13]. The modelling of the freezing/melting processes is based on the previous works but adapted to the novel setup, which is thoroughly described in that paper.

The analytical modelling approach provides a computationally efficient representation of the system dynamics, since the proposed models involve solving low-order differential equations. Nevertheless, as stated in the mentioned work by Bejarano et al., the continuous modelling involving a single inward freezing/melting front within the PCM capsule provides a limited description of the system dynamics: only strict full charging/discharging operations can be simulated [13]. If a realistic representation of the dynamic evolution of the system during any series of partial charging/discharging operations was intended, in such a way that an arbitrary number of moving freezing/melting boundaries could be present at the same time inside the PCM capsules, this would mean a potentially infinite-dimensional state vector. However, keeping in mind that the TES model is intended to be used within a more complex model including the refrigeration cycle, from which efficient energy management strategies are intended to be designed, partial charging/discharging operations dictated by economic and energy efficiency criteria seem likely to be scheduled. Thus, this intrinsic limitation of the analytical models represents a hard-to-overcome drawback.

On the other hand, regarding finite-element methods, Computational Fluid Dynamics (CFD) represent a very common alternative to model the melting and freezing processes taking place in each individual PCM nodule. CFD software packages such as GAMBIT or ANSYS FLUENT are common examples in this context [22].

To keep a reasonable representation of the physical processes taking place at the melting front, model grid density must be high enough to smoothly cover the solid-liquid interface. Diverse mathematical solutions have been studied in the literature [11,23]. The fixed grid approach is able to deal with strong nonlinearities, not requiring explicit treatment of conditions on the phase change boundary, which allows to use standard solution procedures for the energy equations. However, the required high grid density is not needed elsewhere in the numerical domain. Therefore, adaptive grid or front tracking schemes evaluate the exact location of the moving boundary on a grid at each step [24]. There are two main approaches: the interface-fitting grids and the variable-space grids. In the interface-fitting grids (also referred to as variable time step methods), a uniform spatial grid but a non-uniform time step are used. Furthermore, in the variable-space grids, or dynamic grids, the number of time intervals is constant, while the spatial intervals are adjusted in such a way so that the moving boundary lies on a particular grid point, thus the spatial intervals are a function of time. Concerning computational load, it has been widely documented that CFD methods, in general, demand considerable computational resources, being more useful during design stages than to perform continuous simulations over long time periods, typically inherent to energy management strategies.

The authors have proposed a discrete model of the TES system combined with refrigeration cycle in the mentioned recent work, similar to finite-element methods, which has been shown to provide a suitable description of the system dynamics for both, full charging/discharging cycles and any series of partial charging/discharging operations [13]. It is in fact a double-discrete model, since not only it is a time-discrete one, but also a volume quantisation of the PCM nodules is imposed, as the PCM capsules are conceptually divided in a given set of spherical layers. Albeit far below from the expected computing workload of classical CFD implementations, this discrete model is still computationally demanding, apart from the fact that the number of spherical layers represents a trade-off between reduction in modelling errors, with respect to the pure-conduction continuous model presented in the same work, and computational load.

Being aware that the TES model is intended to be used as a component of a global model comprising the refrigeration cycle, from which energy management strategies are to be performed, the computational load must be low enough. In fact, at the top level, where efficient