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Abstract :
The goal of our study is to analyse the performances of a latent heat thermal energy storage (LHTES) solution by modelling its behaviour when considering the thermal and hydraulic phenomena. This work consists in developing and implementing a module dedicated to the resolution of Eulerian (fixed grid) conservation equations for an incompressible fluid in the presence of a phase change where convective motions are present (convection dominated phase change). The model is done by using the free CFD software OpenFOAM. The purpose of this paper is to present some of the results obtained through the use of our modelling tool. Thermophysical properties of the phase change material (PCM) are essential input data for the model. The model allows us to show a preponderance of the good determination of these properties and, in particular, the major role played by the numerical models used to characterize the phase change phenomenon in the prediction of the storage performances.

Keywords :
CFD, Energy Savings, PCM, Thermal Energy Storage.

1. Introduction

The increase of the share of renewable resources, as primary energy in the electricity production process, passes through the lifting of many technological obstacles. Among them, the issue of intermittency of the resource is a crucial one for all the actors in the area. In this context, the increasing use of PCM is done to respond to the problem of smoothing power generation via the establishment of a thermal storage system [1]. Due to large heat storage capacity in the form of latent heat with small temperature variation during heat charge and discharge processes, LHTES solutions appear to be one of the most efficient way to bridge the gap between energy supply and demand. In order to develop this kind of technology, it is crucial to clearly understand all the physicals phenomenon involved during the melting and the solidification processes of the PCM. Because of the non-linear nature of the problem, numerical analysis is necessary to predict the thermal beahaviour of such systems. So the mathematical modelling of the PCM became a tremendous point on which we need to focus to achieve optimal storage design. Several authors have released numericals studies of the performance of such storages [2, 3, 4, 5]. The conclusion that can be done after reading these works is that the precise determination of the intrinsic properties of the used PCM is not often a subject of further analysis. But these properties are essential simulation parameters for a fair determination of the performance of the modeled thermal storage system. The tool presented in this article allows us the simulation of coupled thermal phenomena (heat and mass transfers), in the presence of conduction and convection, of a heat thermal storage system including a latent portion. Here we show the preponderance of a good determination of the properties of the phase change material in the analysis of the performances of a thermal storage device. This analysis is done by modelling the storage by considering the thermal and hydraulic phenomena and especially in the context of this release, through the fill factor.

2. Modelling of the solid/liquid phase change

2.1. The governing equations

The strategy adopted here is based on an Eulerian resolution (fixed mesh) of the conservations equations for an incompressible fluid in the presence of a phase change dominated by convective motions (convection-dominated phase change). In concrete terms, we start from the formulation of the conservation equations which is in the form of the following partial differential equations (PDE) system :

$$\overrightarrow{\nabla} \cdot \left(\rho \overrightarrow{V}\right) = 0 \tag{1}$$

$$\frac{\partial \rho \overrightarrow{V}}{\partial t} + \overrightarrow{\nabla} \cdot \left(\rho \overrightarrow{V} \otimes \overrightarrow{V} + P\overline{\overline{I}}\right) = \overrightarrow{\nabla} \cdot \left(\mu \overrightarrow{\nabla} \overrightarrow{V}\right) - A\overrightarrow{V} + \rho \overrightarrow{g} \tag{2}$$

$$\frac{\partial \rho h}{\partial t} + \overrightarrow{\nabla} \cdot \left(\rho h \overrightarrow{V}\right) = \overrightarrow{\nabla} \cdot \left(k \overrightarrow{\nabla} T\right) \tag{3}$$

nb : it is assumed that all the thermophysical properties (heat capacity, thermal conductivity and viscosity) are independent from the temperature.

Regarding the inclusion of the condition of cancellation of speed as the fluid passes from the liquid to the solid state, the enthalpy method with artificial porosity is used (enthalpy-porosity method) [6]. The basic principle is to assume that the melting front behaves as a porous medium, which involves adding a Darcy-type source term in the equations of momentum. For this one, the solid fraction is involved in the porosity function so as to cancel the velocity when it is equal to one, i.e. in the solid state. In this way, we gradually switch the speed off when going from the liquid phase to the solid phase. In practice, this source term is directly proportional to the velocity and involves the porosity function, which we will detail below.

With the Boussinesq approximation we assume that the density is constant except for the term of buoyancy in the momentum equation (2). The second member is then greatly simplified and involves the new term :

$$\sum \overrightarrow{F}_{\text{vol}} = -\rho g \beta \left(T - T_{\text{ref}}\right) \overrightarrow{e_z} \tag{4}$$

Finally, closing the system of equations (1) à (3) is done by the definition of the state law that links the specific enthalpy with the temperature. We will see below the two thermodynamic models considered in our study for a PCM.

2.2. Thermodynamic closure

The resolution of the previous PDE system means to clarify the relationship $h\left(T\right)$ between the enthalpy and temperature. In this section relations in the case of a pure substance and in the case of a binary solution are presented. First note, the function $h\left(T\right)$ is discontinuous for pure substance so that it is continuous to the mixture (except in the case of eutectic concentration). Furthermore, in the first case, the phase change is characterized by a single temperature T_m and latent heat L_m while in the second it is characterized by a gradual merging on the interval $\left[T_E, T_m\right]$ as we can see on Fig.1.

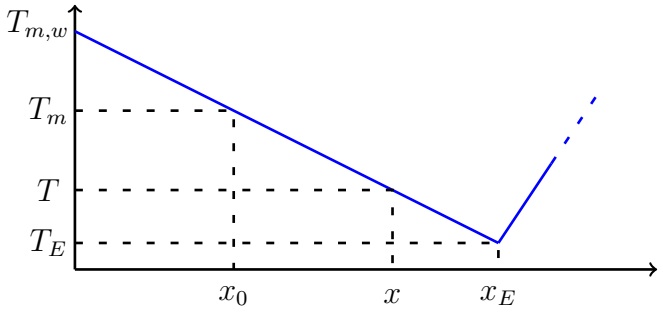


Fig. 1 *Phase diagram for an eutectic solution [7]*

Mathematically, the formulation of the enthalpy for pure body is as follows :

$$h = \begin{cases} h_{\text{ref}} + c_s\,(T - T_{\text{ref}}) & \text{if } T < T_m \\ h_{\text{ref}} + c_s\,(T_m - T_{\text{ref}}) + Y_l\,L_m & \text{if } T = T_m \\ h_{\text{ref}} + c_s\,(T_m - T_{\text{ref}}) + L_m + c_l\,(T - T_m) & \text{if } T > T_m \end{cases} \tag{5}$$

While for a binary solution, it is an expression of the type [8] :

$$h = \begin{cases} h_{\text{ref}} + c_s\,(T - T_E) & \text{if } T \leq T_E \\ h_{\text{ref}} + const1 + (T_{m,w} - T_m)\left(\dfrac{L_{m,w}}{T_{m,w} - T}\right) & \\ \quad + c_s\,(T + (T_{m,w} - T_m)\ln(T_{m,w} - T)) - c_l\,(T_{m,w} - T_m)\ln(T_{m,w} - T) & \text{if } T_E \leq T \leq T_m \\ h_{\text{ref}} + c_l\,(T - T_m) + const2 & \text{if } T > T_m \end{cases} \tag{6}$$

In which :

$$\begin{aligned} const1 \;=\; & L_E - \Big((T_{m,w} - T_m)\left(\frac{L_{m,w}}{T_{m,w} - T_E}\right) + c_s\Big(T_E + (T_{m,w} - T_m)\ln(T_{m,w} - T_E)\Big) \\ & - c_l\,(T_{m,w} - T_m)\ln(T_{m,w} - T_E)\Big) \end{aligned} \tag{7}$$

And :

$$\begin{aligned} const2 \;=\; & c_s\Big(T_m + (T_{m,w} - T_m)\ln(T_{m,w} - T_m)\Big) \\ & - c_l\,(T_{m,w} - T_m)\ln(T_{m,w} - T_m) + const1 \end{aligned} \tag{8}$$

Concerning the expression of the mass fraction of liquid Y_l for the pure substance, it is assumed a linear variation of the form :

$$Y_l = \begin{cases} 0 & \text{if } h < c_s T_m \\ \dfrac{h - c_s T_m}{L_m} & \text{if } c_s T_m \leq h < c_s T_m + L_m \\ 1 & \text{if } h \geq c_s T_m + L_m \end{cases} \tag{9}$$

In the case of the binary solution, we define the liquid mass fraction as follows :

$$Y_l = \begin{cases} 0 & \text{if } h < 0 \\ \dfrac{h}{const2} & \text{if } 0 \leq h < const2 \\ 1 & \text{if } h \geq const2 \end{cases} \tag{10}$$

2.3. Porosity function

Originally, Voller & Prakash [6] proposed the following expression for the porosity function :

$$A = -C \frac{(1-\lambda)^2}{\lambda^3 + q} \tag{11}$$

Where C and q are constants experimentally determined to account for the morphology of the porous medium, and λ the corresponding porosity defined as $\lambda = 1 - Y_s$.

2.4. Numerical resolution

Having defined the PDE system characterizing our problem of a liquid/solid phase change in the presence of convective effects, we are now interested in the numerical method used for its integration. The proposed resolution is therefore done with free software OpenFOAM (`http://www.openfoam.com`), which is a cell-centered finite volume code developed in C++. In version 2.2.1 that we use, the phase transition model that interests us is not available, so we have developed it in order to be implemented in the library of physical models of OpenFOAM. In practice, to solve the PDE system, we have used a PIMPLE formulation, which is a combination of the classical pressure-implicit split-operator (PISO) scheme for the velocity-pressure coupling with the semi-implicit method for pressure-linked equations (SIMPLE) for the pressure discretization.

3. Results

3.1. Test case definition

In the present study, we consider the case of a rectangular storage with a fixed temperature at the lower limit while other walls are adiabatic as shown on Fig.2. We look successively the case of a load, a discharge or a cycle. To represent the PCM, we will consider the thermodynamic closures described above, with two different situations in the case of the binary solution ; in practice, the functions used are those presented in Fig.3. Indeed, it is very common to rely on one or the other of these approaches. On Tables 1 and 2 the thermophysicals properties of the different materials used in our test cases are given. The calculation is done on a common regular grid, whose spatial discretization is 8 mm $\times$ 1 mm.

nb : for convenience, here we represent the test case horizontally but in our simulations we set the gravitational force $\overrightarrow{g}$ such as we simulate a vertical storage device.

To compare the results of the various formulations, we will calculate the load factor (or fill factor). This parameter, often used as a criterion of performance for a thermal storage system, is defined as the ratio of the stored energy (or removed from storage) at a given time over the total storage capacity (or destocking) of the system. We will then present the evolution of the fill factor over time for the various simulations.

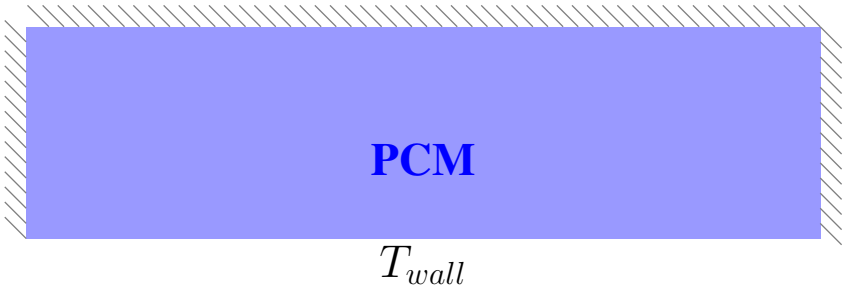


Fig. 2 *Schema of the test case configuration.*

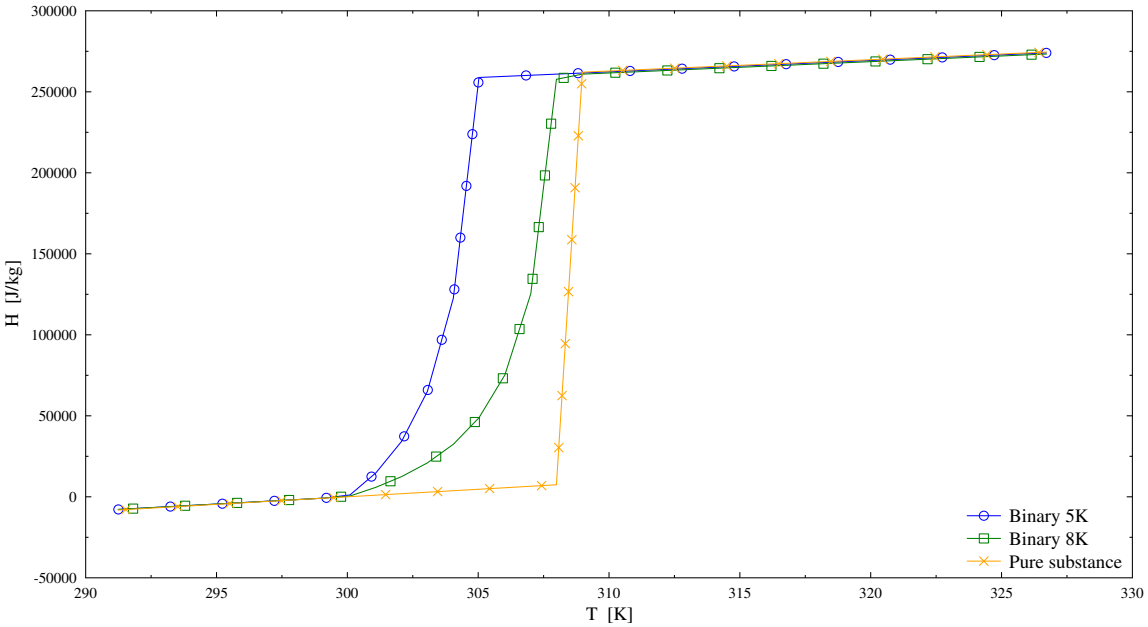


Fig. 3 *Thermodynamic models used for the PCM's enthalpy*

Table 1 *Thermophysicals properties of the pure material.*

ρ	c_s	c_l	k	L_m	T_m	β	ν
820	930	700	0.2	254 000	308.15	$1 \cdot 10^{-3}$	$3.3 \cdot 10^{-6}$

Table 2 *Thermophysical properties of the binary solution.*

Type	ρ	c_s	c_l	k	$L_{m,w}$	$T_{m,w}$	T_m	β	ν	L_E	T_E
Bin5K	820	890	700	0.2	321 000	306.3	305	$1 \cdot 10^{-3}$	$3.3 \cdot 10^{-6}$	0	300
Bin8K	820	890	700	0.2	290 000	309.15	308	$1 \cdot 10^{-3}$	$3.3 \cdot 10^{-6}$	0	300

3.2. Charge and discharge

A charge, respectiveley a discharge, corresponds to a heat supply, resp. recovery, to the storage device. Practically, this means that either a heat flux or an hot temperature (resp. cold) is set to one of the boundary of the system. Consequently, in Fig.4, the results related to the dynamic charge/discharge are presented depending on the model chosen for the PCM for similar physical time. Here the wall temperature is set to an hot value ($T_{wall} = 326.15K$) all along the load step, then its value becomes colder for the unload one ($T_{wall} = 296.15K$).

It is clear that different results are obtained with the various thermodynamical modelling, although these ones may store exactly the same amount of energy since their enthalpy differences are the same on the tested temperature range. Thus, one may, for example, have up to 10% deviation in storage and up to 20% in discharge between the simulation with the pure substance modelling and with the case of binary 5K. The main reason for such a bias comes from the difference in the beginning of the melting for each formulation. Thus, the heat flow rate given to the device is clearly modified since for one temperature, a heat input will not cause the same increase of temperature for each modelling. As an example, the pure substance modelling is stil in the sensible part and therefore it will have a higher increase in temperature than the two other ones wich undergo the transition phase.

Eventually, to fully highlight the possible consequences for an industrial purpose, we propose to also study the fill factor which is a key parameter in the system design process, and where such a gap can clearly compromise the optimal operating conditions.

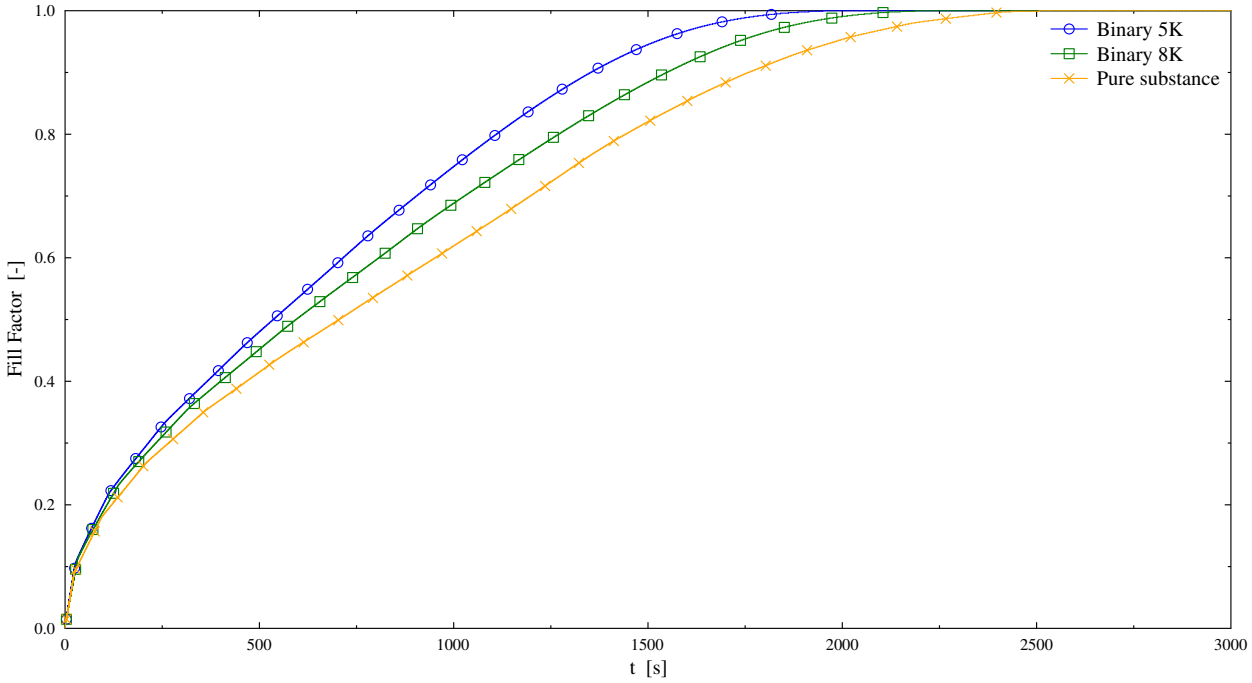
3.3. Cycling

If we now envisage a situation close to the actual operating conditions of these facilities, it is necessary to consider a charge/discharge cycle of the stock. The corresponding simulation results are provided in Fig.5 ; it is clear that depending on how the PCM is modelled, it can lead to an error on the total quantity stored and as a result, on the final value still available at the end of the cycle. Practically, this means that we could stop the storage process before being certain to have completely saturated the system or on the contrary we must maintain the flow of the working fluid beyond the necessary time. Similarly, one can easily imagine that the stock will discharge with a much different dynamic of what was originally planned when the number of cycles increases ; in practice, this could lead to situations where no energy is available, which implies the shutdown of the production.

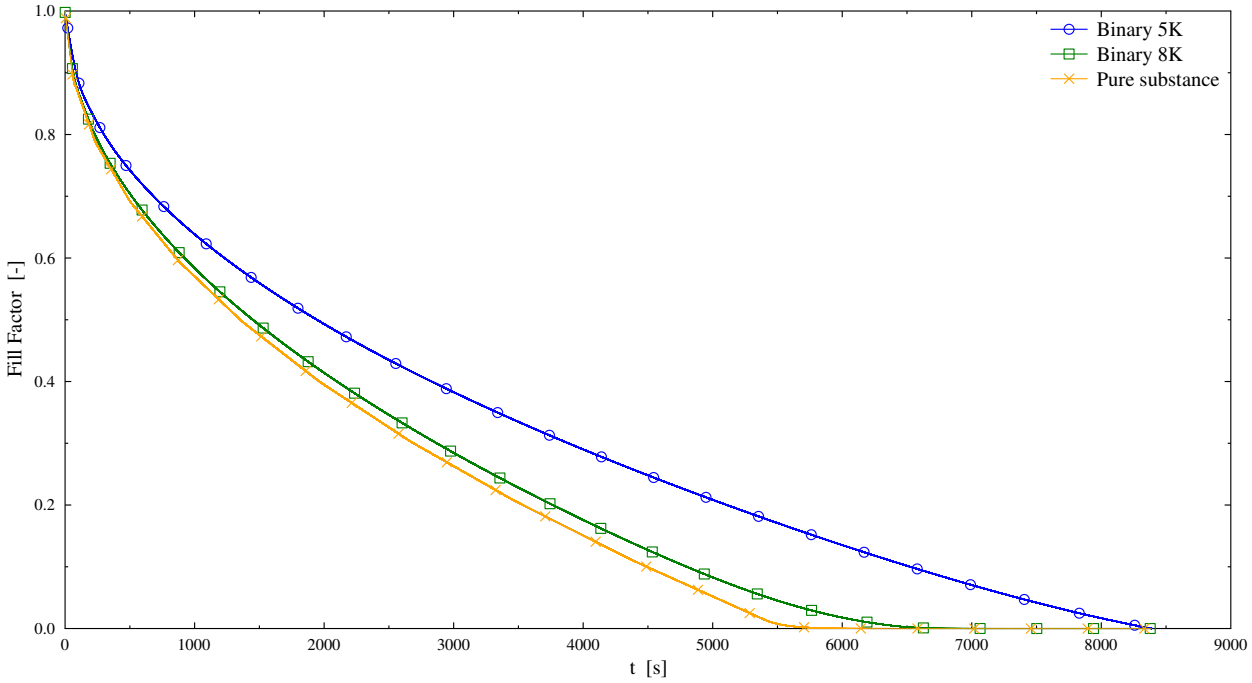
4. Conclusion

Through the analysis of an energy criterion, the fill factor, it has been shown in our study the challenge represented by a good determination of PCM properties in modelling the running of a latent heat thermal storage system. It thus implies that the global performances, as well as the operating conditions, are greatly dependent on this parameter.

The thermodynamical properties of the PCM do not always remain fix through the life cycle of a LHTES. The contact with the metal composing the walls of the exchanger, the series of fusion and solidification processes, all of this may induced an alteration of the PCM's properties. As an example, an experimental campaign led by our laboratory highlighted the fact that after few charge/discharge cycles, the corrosion of metallic materials in contact with the PCM lead to the production of degrated product of the initial material. So we can easily imagine a PCM used in a storage device which initially have the characteristics of a pure material but through

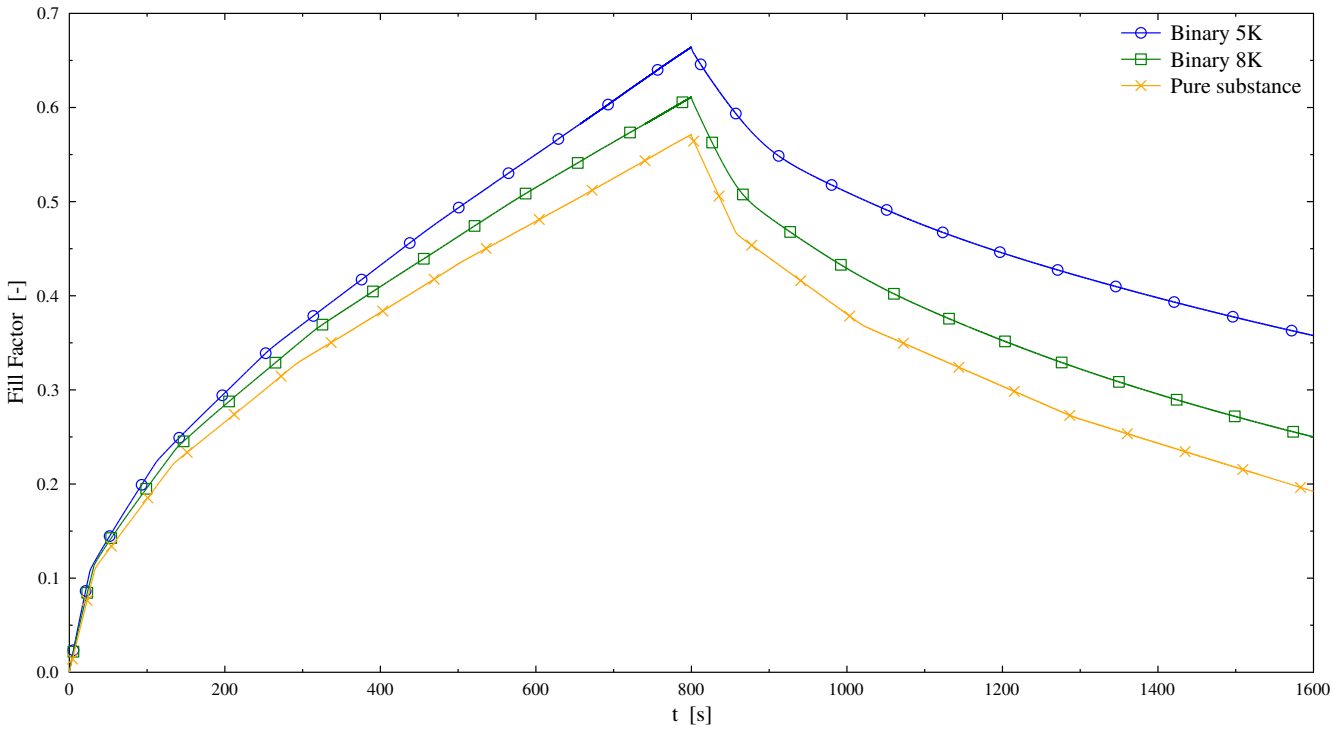


(a) Fill Factor load.



(b) Fill Factor unload.

Fig. 4 *Comparison of fill factor obtained by the thermodynamic model of PCM*



(a) Fill Factor cycled.

Fig. 5 *Fill factor comparison obtained by the thermodynamic model of the PCM at a charge/discharge cycle*

the cycling undergoes degradation of its properties and so have finally the behaviour of a binary.

Eventually, such kind of modelling could predict the global performances of the storage by considering the possible material degradation. But the influence of these thermodynamic parameters is also observed on other variables, for example, when studying the evolution of the melting front and deformation over time induced by convective motions in the liquid phase.

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Nomenclature

Latin letters

A	porosity function, kg/(m^{3}s)
c	specific heat, J/(kg K)
e	thickness, m
g	gravitational force, m/s^2
h	specific enthalpy, J/kg
k	thermal conductivity, W/(K m)
l	length, m
L	latent heat of fusion, J/kg
P	pressure, Pa
r	radius, m
T	temperature, K
$\overrightarrow{V}$	velocity, m/s
x	abscissa coordinate, m
y	ordinate coordinate, m
Y	liquid mass fraction
z	spatial coordinate, m

Greek letters

β	volumetric thermal expansion coefficient, 1/K
ρ	density, kg/m^3
μ	dynamic viscosity, kg/(m s)
ν	kinematic viscosity, m^2/s

Subscripts

E	eutectic
m	melting
l	liquid
liq	liquidus
ref	reference
s	solid
sol	solidus
w	solvent

Abbreviations

PCM phase change material
CFD computational fluid dynamics
LHTES latent heat thermal energy storage

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