Numerical analysis of the solidification process of water used as PCM in a rectangular latent heat thermal storage unit

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Abstract. A numerical analysis of the solidification process of water used as phase change material (PCM) has been carried out in a rectangular latent heat thermal storage unit. The major heat transfer phenomena involved in such a process were numerically characterized using the CFD code Star CCM+. During the solidification process, the flow and heat transfer were analysed through vector field, temperature and solid fractions contours. Quantitative global results such as the temporal evolution of the average temperature of the PCM were also provided during the solidification process. The present study shows that the natural convection plays an important role in heat transfer kinetics during solidification process.

1. Introduction
During the last decades, latent heat thermal storage (LHTS) has gained significant attention because of its high energy density per unit mass/volume at constant temperature. Different configurations of latent heat thermal storage units find their applications in various engineering fields (solar thermal application, passive heating of buildings, air conditioning systems, etc.) [1]. The research studies on LHTS have been generally focusing on the investigation of the overall thermal behaviour and performance. Results show that, during melting, heat is transferred to the PCM first by conduction and later by natural convection. Contrary to melting process, solidification is dominated by conduction. During solidification, natural convection exists in the beginning and as the time goes the effect of natural convection becomes almost zero as compared to the effect of conduction [1]. Hence, whether in fusion or solidification, natural convection has to be taken into consideration. The optimization of LHTS systems requires better quantification and understanding of the heat transfer kinetics taking into consideration the different modes of heat transfer involved in the process of energy storage/release in real industrial systems where storage containers geometries are more complex. CFD techniques are indispensable for the development of more efficient systems. Several recent research articles show that the combination of 3D CFD investigation with experimental validation at lab scale is very promising for the optimisation of LHTS systems [2-3]. In our study, a three-dimensional numerical analysis of the thermal behaviour of a rectangular latent heat thermal storage unit, carried out under transient state conditions, is studied in order to contribute in the optimization of this type of units for agro-food industry. The CFD modelling is made using the commercial code Star CCM + V12.02 [4] with a validation using bibliographic benchmark.

2. Geometry description and boundary conditions
The present study focuses on the numerical analysis of a rectangular LHTS unit as presented in figure 1. A heat transfer fluid flows by forced convection inside the Heat Transfer Fluid (HTF) tube (made of copper), and exchanges heat with the PCM which occupies the outer rectangular tube.

| HTF tube | PCM | PMMA |
|----------|-----|------|
| d_m / d_m | L / d_m | H / d_m | W / d_m | L'/ d_m | H'/ d_m | W'/ d_m | e / d_m |
| 1.071 | 11.43 | 7.14 | 3.57 | 3.57 | 11.43 | 7.86 | 7.86 | 2.14 |

Table 1 : Dimensionless parameters of the rectangular LHTS unit

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The dimensionless parameters of the rectangular LHTS unit (figure 1) are summarized in table 1. The insulation around the PCM (walls of the rectangular LHTS unit) is made of thick PMMA. This material is used for optical reasons; as an experimental test bench is being set up that will later allow a precise evaluation of the solidification front using visualization techniques. In this paper, only the numerical results will be presented.

![Figure 1: Illustration of the rectangular LHTS unit and the grid structure in a transversal plane at the middle of the storage unit](image)

The following initial and boundary conditions are considered during transient state operation. 

**Initial conditions:** At the initial time, the entire computational domain is supposed to be at an initial uniform temperature $T_i(x, y, z, 0) = 4 \, ^\circ C$.

**Boundary conditions:** At the inlet of the cooling HTF, a Poiseuille velocity profile, corresponding to a Reynolds number $Re = 500$ based on the inner diameter of the coil $d_{in}$, is imposed with a constant inlet temperature $T_{in} = -4 \, ^\circ C$. At the outlet of the cooling HTF, a pressure outlet boundary condition is used. At all fluid-solid and solid-solid interfaces, conjugate heat transfer is considered. All the external boundaries of the PMMA walls are adiabatic.

In this study, for the solidification process modelling, the enthalpy approach is adopted, which is widely applied. In order to simplify the mathematical model, the following assumptions are used: (1) The flow of the cooling HTF is modelled through the conservation equations (mass, momentum) in a laminar regime using brine as working fluid which is considered to be incompressible and viscous; (2) the flow of liquid water PCM is assumed to be laminar, unsteady and incompressible; (3) the thermophysical properties of liquid and solid phases of the water PCM, the cooling HTF, the copper and the PMMA are evaluated at an average reference temperature of $0 \, ^\circ C$. (4) The Boussinesq approximation is assumed for the density variation of liquid water PCM in order to take into account natural convection during the solidification process, (5) the viscous dissipation and volume change during solid-liquid phase change are neglected.

**3. Numerical procedure**

The commercial code STAR-CCM + V12.02 [4] was used to solve the conservation equations based on a finite volume discretization method. The conservation equations were solved sequentially using the AMG algebraic solver and the SIMPLE algorithm for pressure-velocity coupling. A second-order
discretization was chosen for the convective terms of the momentum and energy equations. A temporal discretization of second order was chosen.

A grid sensitivity study was carried out for the storage unit configuration by generating several set of grids with refinement in the PCM, and in the vicinity of wall in order to precisely capture velocity and temperature gradients (figure 1). It was finally decided to use the grid with 1 Million of cells taking into account the compromise between precision and available computing resources. Moreover, since the precision of the results is intimately related to the time step chosen for unsteady calculations, a time step sensitivity study was also carried out and this study led to conclusion that the use of a time step of 0.2 s and a maximum inner iteration of 100 was enough to obtain reliable results.

In order to validate capability of the CFD code to model melting/solidification phenomena, an initial run was performed and compared with a reference benchmark solution for phase change with natural convection [5]. Table 2 shows comparison of liquid fraction at different times between our results and the reference benchmark results of Hannoun et al. [5]. The results of present calculation are in good agreement with the benchmark solution.

| Time(s) | (a) Liquid fraction (Benchmark results) | (b) Liquid fraction (Numerical results) | Relative error (%) |
|---------|----------------------------------------|----------------------------------------|--------------------|
| t=100s  | 0.089                                   | 0.089                                  | 0%                 |
| t=300s  | 0.156                                   | 0.157                                  | 0.6%               |
| t=700s  | 0.254                                   | 0.256                                  | 0.79%              |

4. Results
In this section, quantitative and qualitative results are presented. Figure 2 shows the temporal evolution of the solidification front (ice growth) in a transversal plane at the middle of the storage unit (PCM side) during solidification process. It can be noticed that the ice formation is not axisymmetric. This indicates that, conduction is not the only heat transfer mechanism involved in the process. The asymmetry of the ice growth is more likely due to the effects of natural convection.

![Figure 2](image)

Figure 2: Temporal evolution of the solidification front in a transverse plan at the middle of the storage unit on the PCM side

Over time, solidified layers surround and accumulate on the heat transfer surface. It can also be seen that the ice thickness is greater on the upper side of the heat transfer surface than the lower side.
In order to deeply highlight and analyse the effect of natural convection during the solidification process, figure 3 shows the velocity vectors over time in a transverse plane at the middle of the storage unit on the PCM side during the solidification process and the corresponding temperature contours. The presence of rolling cells clearly highlights the development of natural convection which is most noticeable at earlier stages of the solidification process (Figure 3a). With the course of time, as the ice grows, the effect of natural convection decreases up to become negligible. The temperature gradients are higher at the beginning of the solidification process where natural convection is more important (figure 3b). The highest temperatures levels are found in the lower part of the PCM. This is due to the fact that the thermal expansion coefficient of water for temperatures below 4 °C is negative. It can be noticed that, over time, isotherms in ice are almost parallel to the heat transfer surface. During solidification, natural convection is important at the beginning and as the time goes, the effect of natural convection decreases up to become negligible in contrast that of conduction.

In order to quantitatively determine whether natural convection has a major role in the solidification process or not, a comparative study of the temporal evolution of the PCM average temperature was carried out for two distinct cases: a first case taking into account the natural convection and a second case without considering natural convection during the solidification process.

Figure 4 clearly shows that the difference in the PCM average temperature is significant between the two cases, in particular during the first 20 minutes, reaching a maximum difference of 16.26% of the maximal temperature gradient in the PCM (8 °C) after 9 minutes when the natural convection is predominant. After this peak, the difference gradually decreases up to become zero whereas conduction becomes the predominant mechanism in the course of solidification.

5. Conclusions
This study was carried out in order to analyse the major phenomena involved in the solidification process of water in a rectangular LHTS unit. The results clearly show that natural convection plays an important role in the solidification process, especially at the early stages of the process, and its effect
decreases over time. Natural convection effects are found to be negligible at the end of solidification. In fact, over time, the solidification isotherms are almost parallel to the heat transfer surface and solidified layers take the same shape as the heat transfer surface. It is important to note that the dimensions of the unit (the tube containing the HTF fluid and the rectangular tube containing the PCM) play an important role in solidification process. In futures studies, the effect of natural convection will be enhanced using surface extension inside the PCM. An experimental test bench based on the present study is being mounted in order to validate the numerical results.

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