Solid-Liquid Phase Change Simulation Applied to a Cylindrical Latent Heat Energy Storage System

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Abstract: One way of storing thermal energy is through the use of latent heat energy storage systems. One such system, composed of a cylindrical container filled with paraffin wax, through which a copper pipe carrying hot water is inserted, is presented in this paper. It is shown that the physical processes encountered in the flow of water, the heat transfer by conduction and convection, and the phase change behavior of the phase change material can be modeled numerically using COMSOL Multiphysics.

The appearance and the behavior of the melting front can be simulated by modifying the specific heat of the PCM to account for the increased amount of energy, in the form of latent heat of fusion, needed to melt the PCM over its melting temperature range. The effects if adding fins to the system is also studied, as well as the effects of the water inlet velocity.

Keywords: Phase Change Material, Melting, Thermal Energy Storage, Fins, Heat Conduction.

1. Introduction

Thermal energy storage (TES) can refer to a number of technologies that store energy in a thermal reservoir for later use. They can be employed to balance energy demand on a daily basis, between day time and night time, which will be primordial for wide scale use of solar energy [1]; or balance energy, through long term storage, over a year [2].

TES has various domestic, industrial and power generation applications and it is a useful way of cutting costs and overall electricity demand. As a result, this technology is becoming more applicable to a wide range of heating, ventilation and air-conditioning systems due to the fact that it can dramatically help reduce energy cost [3]. TES applications include passive storage in building, thermal protection of food and electronic devices, thermal comfort in vehicles and spacecraft, solar energy thermal storage and heating and sanitary hot water [4].

The three main types of thermal energy storage are sensible, thermochemical and latent [5]. Latent heat energy storage systems (LHESS) are considered "one of the most crucial

energy technologies" [6] and work using the large heat of fusion of phase change materials (PCM) to store thermal energy. LHESS are economical and practical because [4]:

- Latent heat is a few orders of magnitude larger than sensible heat, so much more energy can be stored in a system via phase change compared to simple heating of a substance:
- 2. Latent heat exchange happens over a small temperature range.

In these storage systems, the modes of heat transfer encountered in the melting and solidification of phase change materials (PCM) are conduction, convection and close contact melting [7]. During the charging process (melting), when small volumes of PCM are used inside closed storage devices, conduction is the prevailing mode of heat transfer [8], convection can be neglected; while close contact melting plays an important part only during start-up [9].

An obstacle to the use of solid-liquid phase change processes in energy systems is the typically low thermal conductivity of PCM [10], especially PCM made of organic materials (paraffin wax for example) which typically exhibit rather slow thermal response; as an example, the thermal conductivity of paraffin wax is ~0.21 W/m·K while for cooper, it is of 400 W/m·K. Some of the research in that area concentrates on finding ways of enhancing the thermal conductivity of existing PCM by adding particles with high thermal conductivity [11].

The work presented in this paper concentrates on another way of enhancing the apparent heat transfer properties of PCM from a geometric point of view by properly designing the systems so that they offer optimized surface areas for heat transfer: properly placed fins.

This finite element analysis focuses on the solid-liquid phase change processes taking part in a cylindrical LHESS. Through the study, the influence of fins, placed inside the LHESS, on the overall rate of energy storage and the heat transfer rates in the system are assessed.

2. Geometry

A cylindrical thermal storage device is studied (Fig. 1a) which is composed of an inner copper pipe having a radius, thickness and length of 27 mm, 3 mm and 1400 mm respectively through which hot water flows; the pipe passes through the cylindrical storage device, 1000 mm long and extending to a radius of 300 mm, fill with paraffin wax which is used because of its excellent storage capacity and convenient melting temperature; in addition to its well known thermophysical properties presented in table 1. To complete the assembly, 10 mm of insulation encloses the storage device.

To increase the rate of heat transfer from the thermal fluid in the pipe to the paraffin wax having a very low thermal conductivity, equally spaced annular copper fins extending from the pipe are added to the system; the fin thickness is 5 mm. For the purpose of this work, the effects of adding up to 13 fins are studied (Fig. 1b). The effects of changing the hot water flow rate on the overall heat transfer/energy storage process and the melting behavior of the paraffin wax is also studied.

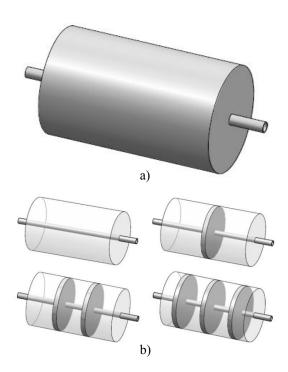


Figure 1. a) Thermal storage device, b) Configuration based on the number of fins.

Table 1. Thermophysical properties of paraffin wax

Thermal Conductivity	0.21 W/m·K
Heat Capacity	2.5 kJ/kg·K
Density	900 kg/m^3
Enthalpy of Fusion	174 kJ/kg
Melting Temperature Range	313 K to 316 K

3. Use of COMSOL Multiphysics

The purpose of this study is to optimize the number of fins needed to completely melt the paraffin wax during a 12 hour charging period, which is typical of a daily charging period when the LHESS is used with a solar thermal collector. The effects of the hot water inlet temperature and velocity will also be considered.

3.1 Governing Equations

Four physical processes have to be simulated in order to study the entire energy storage processes happening inside the LHESS: fluid flow, heat transfer by conduction and convection, and phase change heat transfer. This section presents a summary of the equations needed to account for all four processes.

1. Fluid Flow

In order to simulate the dynamic behavior of the water flowing inside the copper pipe found in the LHESS, the continuity equation, as well as the Navier-Stokes equation, have to be solved simultaneously. The continuity equation takes the following form:

$$\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot (\rho \vec{v}) = 0 \tag{1}$$

where ρ is the density of the water and \vec{v} is the velocity vector.

The necessary Navier-Stokes equation in cylindrical coordinates, accounting for the conservation of momentum, is given by:

$$\rho \frac{D\vec{v}}{Dt} = -\vec{\nabla}P + \mu \nabla^2 \vec{v} \tag{2}$$

where P is the pressure in the fluid and μ is the viscosity of the water.

2. Heat Transfer: convection

Heat transfer from the water to the wall of the pipe happens by convection. In that case, the complete energy equation has to be solved for using the velocities found from the solutions of Eq.(1) and (2). The energy equation describing this heat transfer process is given by:

$$\rho c_P \frac{DT}{Dt} = k \nabla^2 T \tag{3}$$

where c_P is the specific heat of the material, k is the thermal conductivity of the material and T is the temperature. The effect of convection on the heat transfer process is taking care of in the material derivative term DT/Dt of Eq. (3).

3. Heat Transfer: conduction

Heat transfer in the rest of the LHESS is by conduction only. Since the volume of PCM used in between the fins of the system is small, it can be assumed that the effect of convection in the melted PCM is negligible [8]. In that case, the heat conduction equation as to be solved:

$$\rho c_P \frac{\partial T}{\partial t} = k \nabla^2 T \tag{4}$$

4. Phase change heat transfer

In order to account for the phase change process happening when the PCM is melting, the following equation should be solved at the melting interface:

$$k_S \vec{\nabla} T_S - k_l \vec{\nabla} T_l = \rho L \frac{dX}{dt}$$
 (5)

where the subscripts s and l stand for the solid and liquid phase, L is the latent heat (enthalpy) of fusion, and X is the position of the melting interface. Eq. (5) was not solved using COMSOL, a different equation was used to account for the melting process; it will be presented in subsection 3.3.

3.2 Geometry and Boundary Conditions

To perform this numerical study using COMSOL Multiphysics, an axial symmetry (2D) geometry is chosen; and to account for the time

dependency of the problem as well as for the water flow and the heat transfer in the entire system (water, copper, insulation and paraffin wax), a transient analysis under fluid-thermal interaction is used, which enables us to solve both the Navier-Stokes equation and the energy equation for conduction and convection (only in the water).

The geometry presented in Fig. 2 is then created using the following initial and boundary conditions:

- i. Initial temperature of the entire system is 293 K;
- All the outside walls are thermally insulated;
- iii. No-slip conditions on the pipe surfaces;
- iv. No viscous stress and convective flux on the pipe outlet;
- v. Inlet temperature of the water of 350 K and varying water velocity at the pipe inlet between 0.01 and 1 m/s.

3.3 Numerical Resolution

One major problem has to be dealt with: taking into account the phase change process, i.e., accounting for the melting interface and the large amount of energy needed to melt the paraffin wax. Instead of solving for Eq. (5), this problem is dealt with by introducing a discontinuity in the

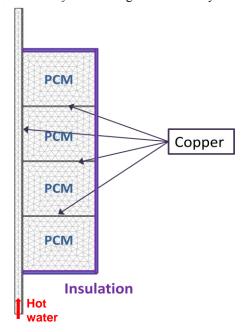


Figure 2. Numerical modeling and meshing of the geometry studied.

specific heat C_P of the material. Using a paraffin wax that has an enthalpy of fusion of 174 kJ/kg and melts over a 3 K temperature range (from 313 K to 316 K), the specific heat of the paraffin wax is modified in the following way:

$$C_p = \begin{cases} 2.5 \text{ kJ/kg} & \text{for } T < 313 \text{ K} \\ 60.5 \text{ kJ/kg} & \text{for } 313 \text{ K} < T < 316 \text{K} \text{ (6)} \\ 2.5 \text{ kJ/kg} & \text{for } T > 316 \text{K} \end{cases}$$

Accounting for this discontinuity is done in two ways by creating functions in COMSOL. The first method uses logic functions which translate into:

$$C_{p_l} = (2.5 + 60.5 * (313 < T) - 60.5 * (T > 316))kJ/kg$$
 (7)

The second method uses the continuous step functions defined in COMSOL as:

$$C_{p_s} = (2.5 + 60.5 \cdot (\text{flc2hs}(T - 313, 0.2) - \text{flc2hs}(T - 316, 0.2)))\text{kJ/kg}$$
 (8)

where flc2hs is a smoothed Heaviside function with a continuous 2^{nd} derivative without overshoot. In order to properly simulate this change in C_p , small and fixed time steps (maximum of 400 seconds) have to be taken to perform the transient simulation. No noticeable difference has been observed between these two methods.

The resulting specific heat C_P of the paraffin wax over the temperature range encountered in the simulation (293 K to 350 K) is presented on Fig. 3.

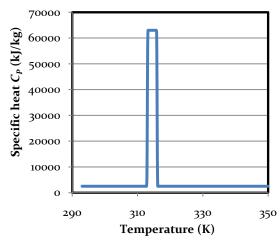


Figure 3. Modified C_P of the paraffin wax.

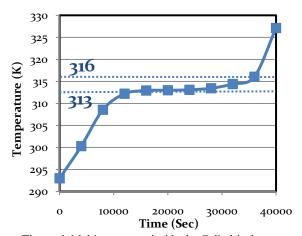


Figure 4. Melting process inside the Cylindrical LHESS.

4. Results and Discussion

Figure 4 clearly shows melting taking place in the PCM inside the LHESS. During the charging process, once the temperature of the paraffin wax reaches 313 K, melting starts which require a larger amount of energy. This can be readily observed from Fig. 4 from the plateau between temperatures 313 K and 316 K, corresponding to the melting temperature range.

Figure 5 presents the temperature distribution inside the cylindrical LHESS after 12 hours of constant charging when 0, 5, 10 and 13 fins are used, inlet velocity of 1 m/s. As can be seen from this figure, the number of fins plays an important role on the overall charging and melting process. Complete melting of the paraffin wax is observed when 13 fins are used, but only in one of the compartments. As expected, there is a higher rate of heat transfer closer to the inlet, which calls for a non-uniform disposition of fins, something that will be addressed in the near future.

Figure 6 presents the PCM temperature as a function of the radius for various numbers of fins. The temperature was taken in the middle of the most energetic compartment in the LHESS (notice the red line in the middle of the most energetic compartment on Fig. 5). It can be observed from this figure that melting will occur close to the pipe regardless of the number of fins.

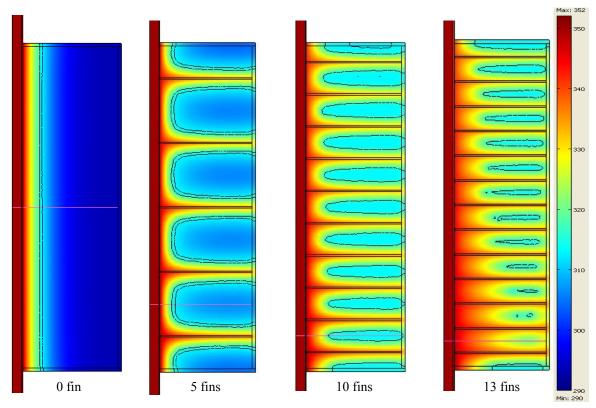


Figure 5. Temperature distribution obtained after 12 hours of charging with an inlet velocity of 1 m/s. The melting interface is represented with black contours.

However, because of the low thermal conductivity of the PCM (paraffin), a minimum

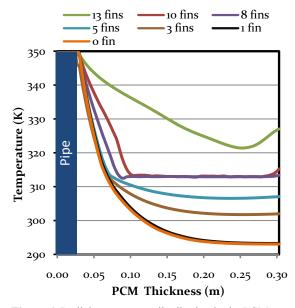


Figure 6. Radial temperature distribution in the PCM found in the most energetic compartment for various numbers of fins.

of 8 fins are required to ensure that all the PCM will at least reach its melting temperature. With 13 fins, all the PCM in the most energetic compartment has melting since the smallest computed temperature in that case is bigger than 316 K. However, from Fig. 5, it is observed that the PCM melted completely only in this compartment which is found close to the inlet where the heat transfer from the water to the LHESS is maximum.

Figure 7 presents the temperature distribution inside a LHESS with 13 fins for various water inlet velocities: 0.01, 0.1, 0.3 and 0.6 m/s. The result for an inlet velocity of 1 m/s is already presented in Fig. 5. It can be observed that, as expected, faster inlet velocities result in higher rates of heat transfer, and larger fractions of melted PCM. However, regardless of the velocity, the size of the region near the inlet where heat transfer is more important does not vary greatly; the size of this region seems to be restricted to 5 or 6 compartments, or approximately the front 35 to 40% of the LHESS.

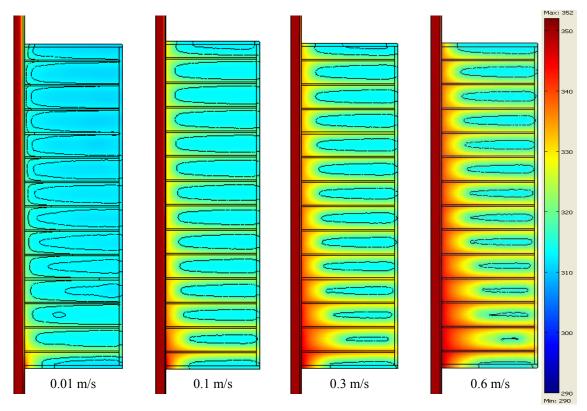


Figure 7. Temperature distribution obtained after 12 hours of charging using 13 fins with various inlet velocities. The melting interface is represented with black contours.

Figure 8 presents the radial temperature distribution, taken in the middle of the first compartment of the 13 fins LHESS presented on Fig. 7, as a function of the water inlet velocity.

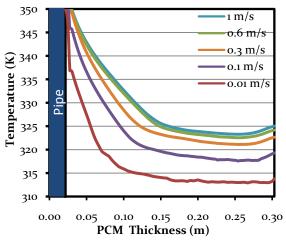


Figure 8. Radial temperature distribution in the PCM found in the first compartment of a 13 fins LHESS for various water inlet velocity.

For the two smallest velocities of 0.01 and 0.1 m/s, the temperature of the PCM is still within its melting range. It can be observed, especially from the temperature distribution of the 0.01 m/s inlet velocity, that some numerical instabilities still persist when heat transfer is calculated at, or close, to the melting temperature range specified for this particular PCM (paraffin wax).

Also, the difference in the attained temperature is relatively small when comparing the results obtained with inlet velocities of 0.6 and 1 m/s. Future simulations will be performed at velocities higher than 1 m/s to see if any noticeable increase in heat transfer can still be gain in that case.

5. Conclusion

This work shows that the physical processes encountered in the flow of water, the heat transfer by conduction and convection, and the phase change behavior of the PCM can be modeled numerically using COMSOL Multiphysics.

The appearance and the behavior of the melting front can be simulated by modifying the specific heat of the PCM to account for the increased amount of energy, in the form of latent heat of fusion, needed to melt the PCM over its melting temperature range.

A complete validation study is currently under way in the authors' laboratory at Dalhousie University. The fluid mechanics, heat transfer and phase change processes encountered in the studied system will all be validated separately using know analytical solutions.

Future works include studying the numerical instabilities encountered when COMSOL is working at temperatures close to the melting temperature range of the PCM and finding ways to reduce them; as well as performing an experimental validation of the numerical results obtained.

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7. Acknowledgements

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