Experimental and numerical comparison of bio-based and conventional phase change materials for thermal storage applications

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Abstract. In the paper, the performance of two phase change materials (PCMs) is evaluated numerically and experimentally. Technical requirements, size limitations and time response of the PCM present crucial boundary conditions when choosing the right material and storage type in the residential sector. The latent heat thermal energy storage system analysed in this paper is a modified shell-and-tube type of heat exchanger using paraffin wax RT-28-HC and a bio-based substance PureTemp28 as phase change materials with heat storage capacity of 255 and 190 kJ/kg, respectively. Their phase change transition temperatures are between 27 and 29°C which makes them suitable for domestic applications together with underfloor heating and heat pump units. In order to properly validate the simulation results, a corresponding machine with the similar initial and boundary conditions has been set up. Additionally, to account for all possible impacts on the performance of the PCM, thermal storage unit was equipped with 24 radially distributed temperature sensors, a pump with variable rotational speed and a water supply machine that operates in temperature ranges from -50 to 150°C. The results from the experiment exhibit very good correlation with the numerical simulations concerning the charging and discharging times.

1. Introduction

As of Paris Agreement in 2015, increasingly more important and rigid requirements are being set to limit the concentration of greenhouse gasses from conventional energy sources. In order to achieve that goal, redundant over-produced thermal energy in the residential sector and power plants should be stored in large quantities into thermal storage units for later use. Sharma and Tyagi [1] investigated the properties of different PCMs under various boundary conditions. They classified the PCMs into three main subgroups: Organic, Inorganic and Eutectic. In this paper a paraffin wax (organic) and PureTemp28 (non-paraffin organic) are investigated experimentally and validated numerically. The latent heat storage (LHS) is based on the absorption or release heat when a storage material undergoes a phase change from solid to liquid or vice versa. The storage capacity of the LHS system with a PCM medium is given by [1, 2]:

\[ \text{Storage Capacity} = \int_{T_{m1}}^{T_{m2}} \frac{C_p}{T} \, dT \]

where \( T_{m1} \) and \( T_{m2} \) are the lower and upper limits of the temperature range, respectively, and \( C_p \) is the heat capacity of the PCM.
\[ Q = \int_{T_i}^{T_m} mC_p \, dT + ma_m \Delta h_m + \int_{T_m}^{T_f} mC_p \, dT \]

\[ Q = m \left[ C_{s,p} (T_m - T_i) + a_m \Delta h_m + C_{l,p} (T_f - T_m) \right] \]

Where \( T_i, T_m \) and \( T_f \) represent the initial, transitional and final temperature during a phase change process, respectively. \( h_m \) is the enthalpy of the PCM in a transitional state. The development of a latent heat thermal energy storage system involves the understanding of three essential subjects: phase change materials, containers materials and heat exchangers [1, 3, 4]. In the developed numerical model, 3 geometrical parameters were varied: length of the pipe, number of the pipes where the heat transfer fluid (HTF) is flowing through and the radius of the pipe. Simulated reference model that was validated with the experiment had the parameters listed in table 1, while the 3D view of the model is shown in figure 1.

| Table 1. Initial and boundary conditions. |
|------------------------------------------|
| Parameter | Amount | Unit |
| \( m_{HTF} \) | 0.05 – 0.0833 | kg/s |
| \( L (z) \) | 1 | m |
| \( r_0 \) | 0.033 | m |
| \( R \) | 0.128 | m |
| \( Np \) | 1 | - |
| \( T_0 \) for HTF and the PCM | 20 (293.15) | °C (K) |
| \( T_{HTF} - \text{charging} \) | 50 (323.15) | °C (K) |
| \( T_{HTF} - \text{discharging} \) | 10 (283.15) | °C (K) |

\( ^1 \) Inner and outer radius
\( ^2 \) Number of nodes in the numerical simulation
\( ^3 \) Number of pipes

(a) (b)

**Figure 1.** 3D view of the latent thermal storage taken as a base geometry for numerical modelling: One shell and tube pipe (a); Thermal storage containing 43 pipes (b).
2. Mathematical and numerical model

Predicting the behavior of phase change materials is difficult due to its non-linear nature at moving phase change interface and due to the presence of different thermo-physical properties in all three phases: solid, liquid and transitional [5]. Numerical approach for solving the PCM melting and solidifying process was based on solving the moving boundary problem equations. The presence of moving boundary in the PCM is implying that the solution of heat and mass balance equations in every time step has to be met. In the present paper the enthalpy formulation for solving the moving boundary problem was used. Since this problem is difficult to solve analytically, finite volume approach with central difference integration scheme for second order differential equations was used.

The latent heat storage unit (LHSU) consists of insulation material, outer and inner tubes. The HTF is flowing through the heat transfer pipe and exchanges heat with the PCM that surrounds the inner tubes. In order to simplify the mathematical model, following assumptions were made:

- The impact of the tube thickness, i.e. the thermal resistance of the tube on the overall melting and solidification is negligible,
- The HTF is incompressible and can be considered as a Newtonian fluid (small mass flow and pressure drops),
- The PCM is isotropic and homogenous,
- The HTF flow is kept in laminar layer,
- The initial temperature of the PCM material is uniform (solid phase – melting and liquid phase - solidification),
- The problem is axisymmetric, HTF, tube wall and PCM temperature variations in an angular direction are assumed to be negligible,
- Natural convection in the liquid phase of the PCM material has been neglected.

2.1. Charging mode

Heat transfer equations for flowing water (HTF) and the PCM are [6]:

For HTF:

\[
\rho C_p \frac{\partial T_f}{\partial t} = - \left( \dot{m} C_p \frac{dT_f}{dz} + (T_{in} - T_f) \pi r_0 \frac{\partial T}{\partial r} \right)
\]  

(3)

For PCM:

\[
\left( \rho C_p \right)_{PCM} \frac{\partial T}{\partial t} = \text{div} \left( k_p \text{grad} \ T \right)
\]

(4)

With the phase change range conditions as follows [6]:

\[
h(t) = \begin{cases} 
C_{p,s} T & T < T_{m1} \\
C_{p,s} T + \frac{\Delta H (T - T_{m1})}{\Delta T_m} & \text{when } T_{m1} < T < T_{m2} \\
C_{p,l} T + \Delta H & T > T_{m2}
\end{cases}
\]

(5)

In the discharging cycle, behavior of the latent thermal storage unit is governed by the same equations as in the charging mode. After inserting the conservation equations (energy and temperature) in a single finite volume element, a heat transfer equation is obtained [6]:
\[
\rho V_j \frac{\partial h}{\partial t} = k_p A_k \frac{\partial T}{\partial R_k} - k_p A_{k-1} \frac{\partial T}{\partial R_{k-1}} + k_p A_j \frac{\partial T}{\partial Z_j} - k_p A_{j-1} \frac{\partial T}{\partial Z_{j-1}}
\]

Equation (6) was then expanded with the discretized spatial and temporal equations and the initial and boundary conditions are added.

2.2. Simulation results

In the following table, phase change material specifications of two different substances are listed. These specifications served as input data for the calculation and calibration of the numerical model. In this paper, the emphasis is not only on the validation of the numerical model but on the performance comparison of two commercially available PCMs as well. The validation of the model was performed on one charging cycle with the properties of RT 28 HC taken from table 2. The temperature was monitored in several coaxial planes parallel to the HTF pipe during charging cycle. Temperature state of the PCM over time is shown on the figure 2.

![Figure 2. Temperature distribution of PureTemp28 at different coaxial planes in time.](image)

**Table 2. PCM specifications.**

| Parameter                      | RT 28 HC | PureTemp 28 | Unit     |
|--------------------------------|----------|-------------|----------|
| Melting point (zone)           | 27-29    | 28          | °C       |
| Heat Storage Capacity          | 250 (± 7.5%) | 190          | kJ(kg)^{-1} |
| Thermal Conductivity (liquid)  | 0.2      | 0.15        | W(mK)^{-1} |
| Thermal Conductivity (Solid)   |          | 0.25        | W(mK)^{-1} |
| Density (liquid)               | 770      | 860         | kg(m3)^{-1} |
| Density (solid)                | 880      | 950         | kg(m3)^{-1} |
| Specific Heat (liquid)         |          | 2.54        | KJ(kgK)^{-1} |
| Specific Heat (solid)          |          | 2.34        | KJ(kgK)^{-1} |
3. Experimental investigation

Figure 3. Schematic view of the latent heat storage test unit.

In order to properly validate the simulation results from Matlab, a corresponding test setup with the similar initial and boundary conditions was designed in the laboratory. The test rig consists of two three-way valves regulating the hot and cold circuit, a mixing unit regulating the inlet temperature, vessel for depressurization in the case of emergencies, two water tanks, the LHSU and the JULABO machine for water supply. Next to those three way valves which are being digitally regulated, four manually regulated two-way security valves were added additionally. The first pair is positioned on the inlet and outlet pipe of the LHSU and the rest at the inlet and outlet of the JULABO machine. The water tanks are made of stainless steel and can be filled up to 600 L. Hot circuit represents the charging cycle where the heat is transferred from the HTF to PCM, i.e. the material is storing heat. The discharging cycle is represented by the cold circuit and in this case, the heat is being transferred from the PCM to HTF. The test set-up is outlined in figure 3 and figure 4.

Figure 4. The LHSU used in the experiments (a); cross section of the LHSU drawing (b); top view of the LHSU cross section (c).
4. Comparison and discussion

4.1. Paraffin wax

Experimental investigation indicated useful information which was later used for the calibration of the numerical model. Experimental results of the melting and solidification cycles for Paraffin RT 28 HC with fluid mass flow of 0.05 kg/s are shown in the figures 5a and 5b, respectively. Each curve represents values from a temperature sensor over time. Two temperature values are displayed, one from a sensor on the inlet inner radius and one from the sensor on the outlet outer radius. In this way, the temperature values in the complete spectrum over space and time were obtained. Inlet temperature was held constant at 50 °C.

![Figure 5](image.png)

**Figure 5.** Experimental results of Paraffin wax as PCM – Melting and Solidification cycle.

If the simulation results are compared with the experimental investigation, it can be observed that the elevation in the material temperature due to the natural convection occurs approx. at the same time (Simulation: 3 h; Avg. Experiment: 3.5 h). The simulation results calculated before the actual experiments show good correlation with the test results. We can observe from the green curve in the figure 5c that the material reaches its peak temperature after 4 hours, approximately the same time as in the simulation. As mentioned before, the impact of the fluid mass flow on melting times was investigated. The mass flow was ranged from 0.03 to 0.083 kg/s due to the fact that the working fluid speed is limited to a maximum value of 1.5 m/s (0.083 kg/s) as specified in the Norm DIN 18380. Further on, the mass flow of the heat transfer fluid had a large impact on the dynamics of heat transfer process, which is also shown in the figure 6. By increasing the mass flow of the HTF and the number of pipes in the heat storage, the efficiency and the reaction times will be increased. Additionally, the
inlet temperature plays a key role in the response time. HTF temperature of 50 °C was chosen as the optimal operating temperature in the experimental investigations of Paraffin Wax RT28HC.

Figure 6. Charging cycle of Paraffin wax as PCM and the influence of fluid mass flow on the melting period (Experiment).

4.2. PureTemp 28

In order to compare the Paraffin wax with another phase change material used for thermal energy storage, a bio-based PCM from Puretemp LLC in Minneapolis was investigated. Bio-based materials usually have faster reaction times, and a longer life expectancy. In this case inlet temperature of the working fluid was set to 47°C with a mass flow of 0.0833 kg/s. Figure 7 depicts a temperature variation of various temperature sensors placed along the PCM during charging cycle. The overall melting cycle lasted approximately 4.5 hours.

Figure 7. Charging cycle of PureTemp28 with data from various temperature sensors.

Comparing the Puretemp28 substance with the Paraffin wax, a similar material behavior could be observed concerning the reaction period. However, the temperature elevation due to the natural convection occurs later in time. Different micro granular structure together with slightly different inlet temperature could be the cause of the shift in the phase change period. This behavior of the material and the influence of the inlet temperature was taken into account in numerical code as well. Due to the
complexity of the bio-based materials and its chemical structure, the longevity of the PCM wasn’t taken into account in the simulations. This would require robust experimental tests and UV monitoring of the material through its complete life cycle. Though, Puretemp 28 has passed all requirements regarding life cycle assessment according to RAL, an independent quality assurance association based in Germany that set the standards for PCM quality. Overall, it could be concluded that the simplified numerical model realistically represents the phase change phenomena in these two materials.

References
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