

# Comparison of PCM encapsulation shapes by computational fluid dynamics simulation

## Introduction

The scope of the present paper is to evaluate the influence of encapsulation geometries on the melting behavior of phase change material (PCM). With respect to the implementation in a hybrid thermal energy storage (HTES) for domestic application, using sensible and latent heat storage materials, a numerical model has been setup in the commercial computational fluid dynamics code Star CCM+. Charge or discharge of a sensible heat storage can be described through rise or sink of the materials temperature in its current aggregate state. Latent heat storages in contrast are storing thermal energy with an almost isothermal behavior by using latent heat of the phase change. Therefore, compared to water, 5 to 14 times higher energy density can be achieved. The equation describing the energy capacity can be written as

$$Q_{latent} = \int_{T_i}^{T_m} (m \cdot c_p \cdot \Delta T) + m \cdot \alpha_l \cdot h_{fusion} + \int_{T_s}^{T_f} (m \cdot c_p \cdot \Delta T)$$

The PCM capsules were simulated inside a cubical tank with an edge length of 0.3 m and a total volume of 27 liters. Two cylindrical pipes were added to the bottom and the top as inlet and outlet. The volumetric dimensions of the PCM capsules are given in Table 1. For simplicity, glass was chosen as encapsulation material, with water as a heat transfer fluid (HTF) and commercially available RT44HC paraffin wax by Rubitherm as a PCM. Initial conditions were set to standard conditions (1.013 bar, 298.15K). The inlet conditions were set to a constant mass flow of water at 0.5kg/s and 323.15K. Data concerning temperature, density and solid volume fraction were collected to evaluate the melting behavior. Simulating melting of paraffin wax as a PCM is still a major challenge, because it not only involves fluid flow and heat exchange, but also phase change. The most popular model for phase change simulations is the Volume of fluid model (VOF). It implies that all immiscible fluids in a cell share temperature, pressure and velocity and does not track the solid-liquid interface explicitly, but instead calculates the liquid and solid volume fraction for every cell at each time step. In addition to the VOF model a mushy zone can be applied that treats the solid-liquid interface like a porous media to avoid high convective flow and simulate a two-phase melting section.

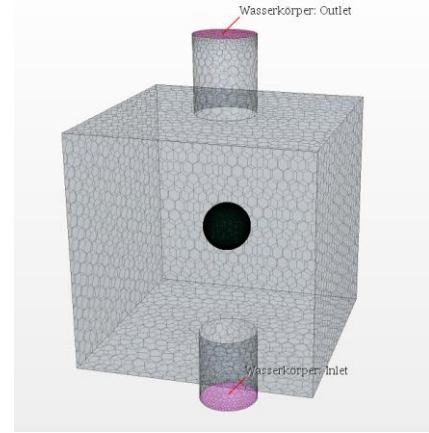
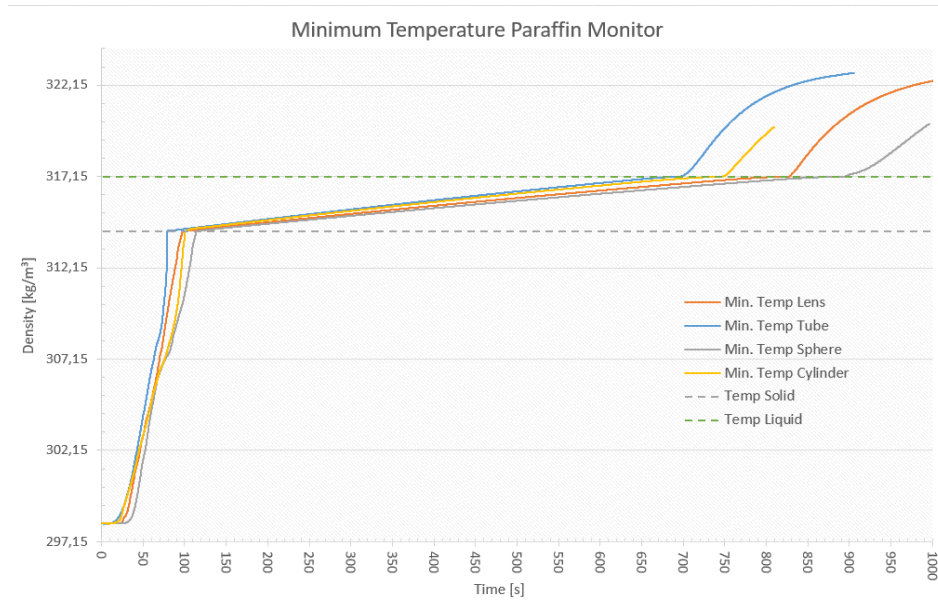


Table 1 - Volumetric properties of simulated PCM modules

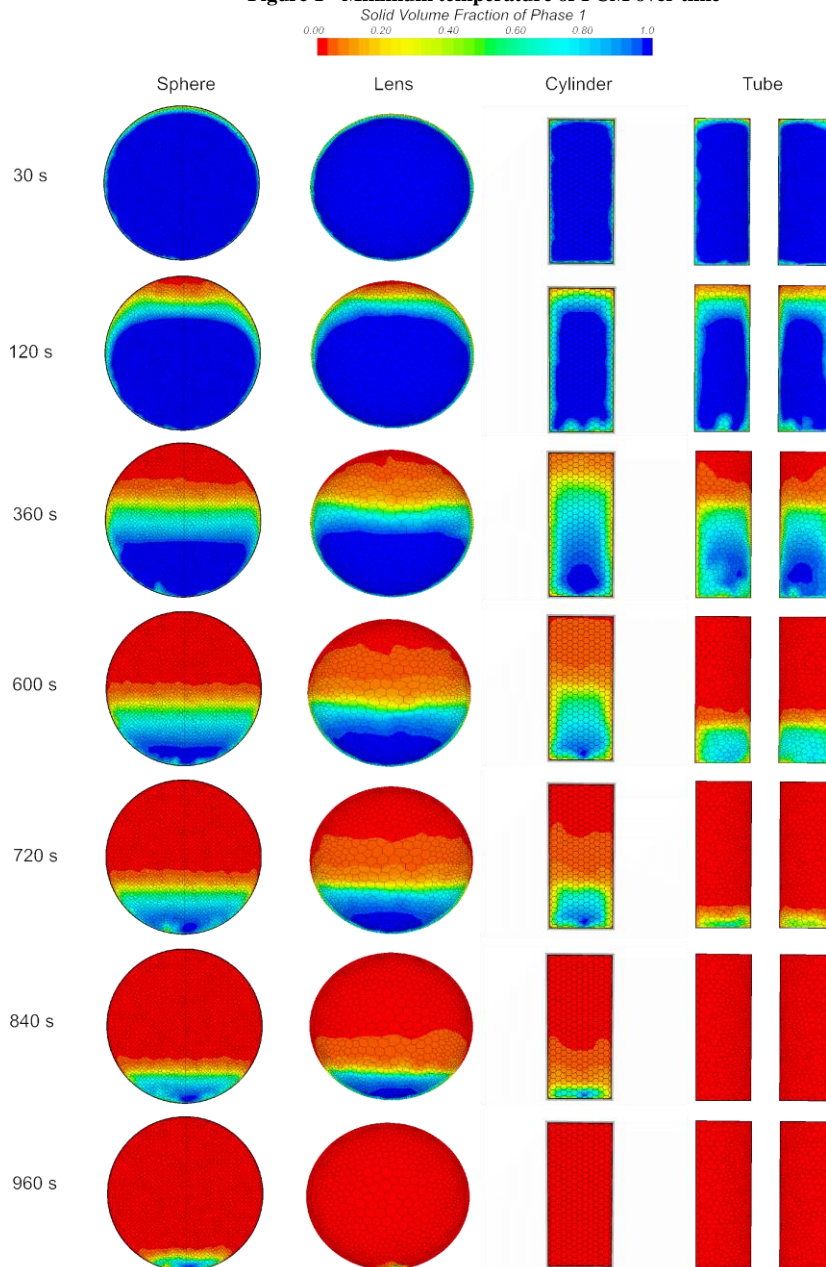
Type		Sphere	Lens	Tube	Cylinder
PCM Volume	[liter]			0.113	
Encapsulation volume	[liter] / [%]	0.012/9.4	0.008/6.5	0.02/14.2	0.014/11.3
Total Volume	[liter]	0.125	0.121	0.133	0.127

## Results

As seen in Figure 1 the temperature profile was very homogeneous. The initial preheating phase (0s to 100s) is marked by the rapid increase of temperature until the PCM reaches the melting temperature. While melting (second phase 100s to 700s), temperature increases gradually until reaching solidification temperature (700s to 900s). The ongoing sensible heating illustrated by the PCM temperature converging the HTF temperature was not within the scope of interest, but necessary to ensure that the paraffin wax is fully molten. It can be clearly seen, that the tubular PCM module was the first to be fully liquified, followed by the cylindrical, the lenticular and finally the spherical module at 692s, 743s, 823s and 886s respectively. Finally, the last simulation run showed the desired behavior presented in Figure 2, where the solid (deep blue) PCM sinks while the liquid (red) material rises to the top of the modules. For use in a domestic hot water storage the tubular module offers the best thermal response due to the large surface, which however leads to high encapsulation volume and therefore decreased storage capacity. In times of low demand and constantly high temperature inside the storage tank, it could even lead to higher standing losses than the less responsive modules.



**Figure 1 - Minimum temperature of PCM over time**



**Figure 2 - Solid volume fraction of PCM during melting process on various time steps**