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Exploring the Properties of User-defined Phase Change Materials for Thermal Energy Storage

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Abstract **-** In this paper, a 2D thermal energy storage (TES) is modelled and solved numerically in the software COMSOL Multiphysics. The aim of this study is to examine the suitability of relevant thermal properties for the selected system design for charging only. The system consists of a cylindrical tank with height 0.5m and diameter 0.5m, acting as a packed bed full of encapsulated phase changing materials (PCM). The heat transfer fluid is water, entering the system at 90°C at a velocity of 0.01m/s. The investigation of the relevant properties focuses on the effect of melting temperature, latent heat of fusion, density, thermal conductivity and specific heat capacity. The final temperatures at different for spheres at different positions across the tank length are recorded and the heat absorbed for said spheres is calculated. Results indicate that the liquid properties of the PCM are more dominant over the temperature reached by system than the solid ones. Furthermore, higher final temperatures have been noted for high thermal conductivity of the liquid. In contrast, high specific heat capacity of the liquid yields significantly lower final temperatures.

Keywords**:** Thermal Energy Storage**,** Latent Heat, Phase Change Material, COMSOL Multiphysics

1. Introduction

As the world progresses into a new decade, it is key that any emerging technologies focus on the challenging issues that are faced in society, including but not limited to climate change and energy consumption/demand. It is no secret that the depletion of fossil fuels is imminent and that renewable systems are required to take their place soon in a smooth transition. Although there are goals in place and the renewable community is growing larger every day, due to the intermittency of their nature, meeting these goals can prove difficult. It is during these times of energy mismatch between consumption and demand that energy storage becomes a necessity more than a commodity. Thus, this paper proposes thermal energy storage as a means of mitigating the problem.

Thermal energy storage (TES) is storing energy in the form of heat. The three main types: sensible heat, latent heat and thermochemical. Sensible heat is the simplest way of storing heat. Essentially, it absorbs or releases heat per degree increased/decreased. It offers several advantages, such as storage high thermal conductivity and low cost [1, 2]. Common requirements include high energy density, good thermal conductivity, good thermal diffusivity, easy manufacturing, low price and stable chemical properties [3]. On the other hand, latent heat absorption happens when a material phase changes, with no temperature variation. It is considered very attractive due to the large amount of heat absorbed and released by the phase change materials (PCM), high storage density and availability for near isothermal systems [4]. Both sensible and latent heat applications can be categorized into low temperature, medium temperature and high temperature. For sensible heat, solids tend to be on the high temperature spectrum, and are combined with many solar renewable applications, where they are combined with mostly molten salts [5]. Further categorisation of latent heat systems materials include paraffin and fatty acids for organic materials, salt hydrates and metallic for inorganic ones and eutectics (which may combine the two) [6]. Due to their large melting temperature ranges which make them available for a wide range of systems and operating temperatures, paraffin and fatty acids have been widely used in TES commercially. Nevertheless, they have the disadvantage of being expensive and having low thermal conductivity values [6]. Inorganics have higher thermal conductivity and latent heat of fusion than organics, yet they pose other issues such as supercooling, corrosion and water formation [6].

Selecting the right material for the system can be challenging, as no material is said to have all favourable and "perfect" qualities without disadvantages. Investigating what other authors have tested in literature can help to identify which material is therefore most suited for a specific application type and will help lessen the drawbacks.

Sivapalan et al. [7] perform an experimental investigation on paraffin wax-water nanoemulsions for use as thermal energy storage media. They selected paraffin wax with a melting point of 58-60°C and used it to create 10 wt%, 20 wt%, 33 wt% and 50 wt% concentrations. Results show that all concentrations except the 50 wt% possess higher specific heat capacity than that of water. Furthermore, these same concentrations had higher thermal conductivity values than pure paraffin wax. Pagkalos et al. [8] analyse and compare water and paraffin as phase change materials for their use in TES. Using ANSYS for computational fluid dynamics, they build a 2D domain which simulates the charging process in two different tube lengths (6.6m and 1m) and two different feed rates (laminar at 30l/h and turbulent at 60l/h). They evaluate the storage material temperature, heat transfer fluid temperature and energy stored. Results indicate using the paraffin PCM stores a higher amount of energy (4.1 more times) but the charging process takes approximately 3.0 to 3.9 times longer. They also experience that a higher flow rate favours a higher heat transfer rate, especially for the paraffin.

Sharma et al. [9] conduct a theoretical investigation on five different fatty acid types, including capric acid, lauric acid, myristic acid, palmitic acid and stearic acid. They propose a 2D simulation model based on the enthalpy approach and calculate the melt fraction using conduction only. They conclude that the thermal conductivity of the material has significant effect on the melt fraction and suggest a careful selection to optimize the performance of the unit. Kant et al. [10] present a study which develops ternary mixtures of fatty acids for low temperature thermal energy storage applications. They combine capric acid (CA), lauric acid (LA), palmitic acid (PA) and stearic acid (SA) into CA-LA-SA (CLS) and CA-PA-SA (CPS), with different weight percentages. These materials are found to have melting temperature in low ranges, such as 14 to 21°C but with good latent heat values. The most promising, CLS, had a melting temperature of 16.41°C and 174.98kJ/kg of latent heat of fusion.

In terms of design, TES systems commonly fall under three categories: single tank, two (or more) tanks and heat exchangers. Tanks are mostly cylindrical ones [11, 12], although some rectangular are reported [13]. Single tanks can be used as packed beds, with thermocline, with heat transfer enhancers, or simply as a single medium storage tank. This paper focuses on a single tank, as it is said to save up to 30% more energy than a two-tank system [14] and also much simpler than a heat exchanger.

Therefore, for tank based systems, the ratio between length (L) or height (H) and diameter (D) is important. Yang et al. [15] state the system cycle efficiency is improved with a larger length ratio and using higher tanks. They also state tank height will affect output temperature directly. Klein et al. [16] test various aspect ratios of 1, 2, 3, 4 and 5 (L/D) for their single tank packed bed. Furthermore, for each aspect ratio, four particle diameters of 10, 16, 25 and 50mm are simulated. Their findings state that for each analysed storage configuration the level of stored energy increased as the aspect ratio increased and the particle diameter decreased.

2. Methodology

This study decided to explore what is the effect of testing and inputting user-defined values for relevant parameters for latent heat TES. These user-defined materials will be encapsulated into "spheres" and simulated in a 2D domain in the software COMSOL Multiphysics. The heat transfer fluid (HTF) will be water, which will heat up the materials until phase change. The selected system design consists of a single tank packed bed and considers the charging aspect only.

The studied parameters were melting temperature, latent heat, density, thermal conductivity (for solid and liquid) and specific heat capacity (for solid and liquid). The results will focus on the charging dynamics, the temperature reached by the PCM and the heat absorption (per sphere). All this is done for the position at the centre of the tank, both vertically and horizontally, which is denoted by the centre sphere. This can help inform what parameters have a greatest effect on the charging dynamics and time of a system with a similar design, which can help and fasten the material selection process, or even offer a change for new materials being used as latent heat mediums where the possibility was not considered before.

2.1. System Design

The system consists of a 2D symmetrical single cylindrical tank domain, of 0.5m in height and diameter (L/D = 1), packed with a set of 19x17 encapsulated spheres containing the user-defined PCM. The tank frame is 0.025m thick and the capsule is considered thin and negligible, with the sphere radius of 0.0125m. There are a single inlet and outlet at the centre of the tank, both 0.12m in length. The HTF (water) enters the system at a constant temperature of 363.15K (90°C) and at a velocity of 0.01m/s. The system initially starts with still water inside the tank surrounding the PCM at an ambient temperature of 293.15K (20°C).

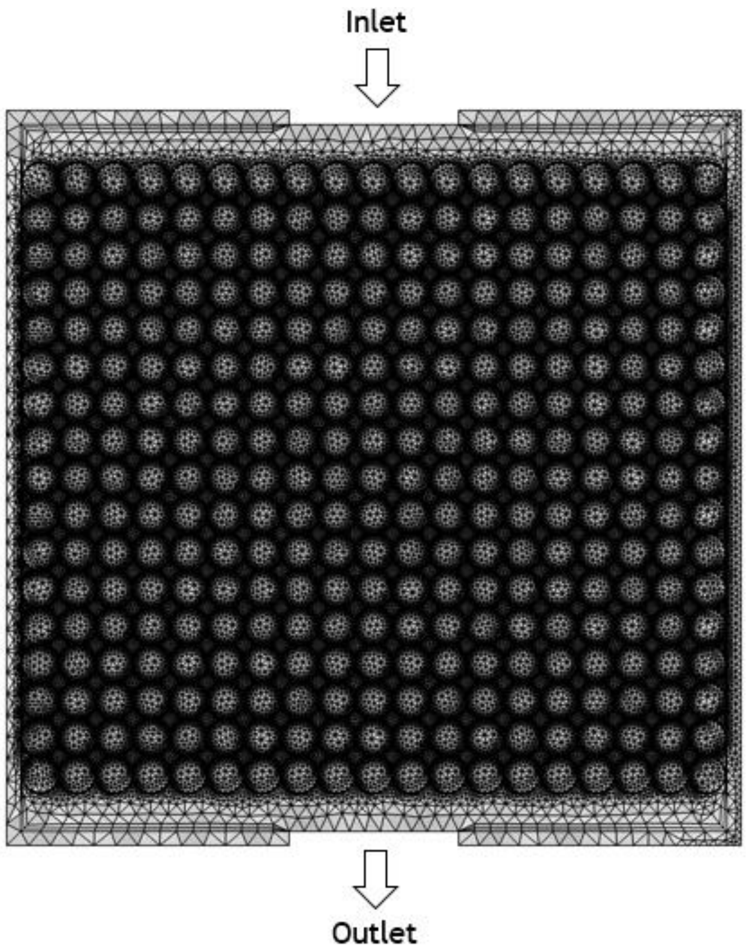

Fig. 1: Physics generated 2D system mesh in software COMSOL Multiphysics.

The mesh seen in Figure 1 is a physics generated mesh composed of approximately 138,000 elements, mostly triangular prisms. The inlet and outlet are clearly marked.

2.2 Boundary conditions and assumptions

The system is an open flow system, modelled in 2D using the software COMSOL Multiphysics. 5.4 The model uses the “Laminar Flow” and “Heat Transfer in Fluids” physics, alongside the “Nonisothermal Flow” multi-physics. Validation of the physics model was carried out based on the system reported in [17]. The mesh is a fine, free triangular mesh with the triangle size being smaller for the spheres than the rest of the tank [18]. The heat transfer problem and temperatures were solved using the heat equation for non-uniform isotropic mediums (1) and Fourier's law (2):

$$\rho C_p \frac{\partial T}{\partial t} + \rho C_p u \cdot \nabla T + \nabla \cdot q = Q + Q_p + Q_{vd} \tag{1}$$

$$q = k \nabla T \tag{2}$$

Where ρ is density, Cp is the heat capacity at constant pressure, T is temperature, t is time, u is velocity, q is the heat flux, Q is the heat source, Qp is heat pressure work, Qvd is heat viscous dissipation and k is the thermal conductivity.

The system is assumed to be perfectly insulated and that there are no thermal losses to radiation (n·q = 0). The inlet is a fully developed velocity profile with weakly compressible flow. The boundary conditions in the wall are no slip and the tangential velocity is equal to zero. On the other hand, the outlet boundary condition is set to pressure, where initial pressure is zero and the model suppresses backflow. All materials tested are assumed to be homogeneous and isotropic. Lastly, the spheres are modelled as circles that do not undergo deformation.

The software will be used to export final temperatures reached by the spheres, and the following equation can then be used to calculate the amount of heat absorbed per sphere for each case:

$$q = m\,(C_{ps} \cdot (T_m - T_i) + L + (T_f - T_m) \cdot C_{pl}) \tag{3}$$

Where m is the mass, Cps is the specific heat capacity of the solid, Tm is the melting temperature of the material, Ti is the initial temperature of the system, L is the latent heat of fusion of the material, Tf is the final temperature reached by the system and Cpl is the specific heat capacity of the liquid.

2.3 User-defined materials

As mentioned previously, the materials tested in this study are not tangible "real" materials, but rather a combination of parameters carefully chosen from previous data in literature. The idea is to vary only one of the selected parameters, whilst keeping everything else constant, allowing to clearly see what that one parameter's influence in the system is. Each simulation was given a code, including the base case which was the reference point for the rest of simulations. The values for the base case and the variations are shown in Table 1:

Table 1: Base case and user-defined material variations for the simulations.

Base Case:	**Variations:**
Melting temperature: 45°C	Melting temperature: 25 to 65°C
Latent heat: 200kJ/kg	Latent heat: 10 to 500kJ/kg
Density: 800kg/m^3	Density: 600 to 1000kg/m^3
Thermal conductivity: Solid: 0.4W/mK Liquid: 0.2W/mK	Thermal conductivity: Solid: 0.1 to 0.4W/mK Liquid: 0.1 to 0.4W/mK
Specific heat capacity: Solid: 2000J/kgK Liquid: 2200J/kgK	Specific heat capacity: Solid: 1000 to 2200J/kgK Liquid: 1000 to 2200J/kgK

3. Results

As mentioned above, all results presented in Figures 2 to 5 below apply to the centre sphere in the tank design. Figures 2 to 4 are analysed in terms of final temperature and Figure 5 is in terms of heat absorbed by the single sphere.

It can be seen in Figure 2 that increasing the melting temperature has a positive outcome on the final temperatures reached, as 65°C not only has a steeper and faster charging time, but also reaches approximately 5K higher than the 25°C melting point one. The 25°C test also has an initial lag of under 100 seconds (from approximately 50s to 150s) before it starts heating up quickly and the gradient becomes steep. The other two tests do not experience this slow charging start. Heating dynamics leading up to phase change also differ from the three tests, and the phase change points are clearly denoted from the flatter sections. Otherwise, the heating dynamics after phase change remain similar as seen by the parallel lines. It is also worth mentioning that after 10 minutes none of the simulations had the centre sphere reach the maximum temperature of the HTF of 363.15K (90°C).

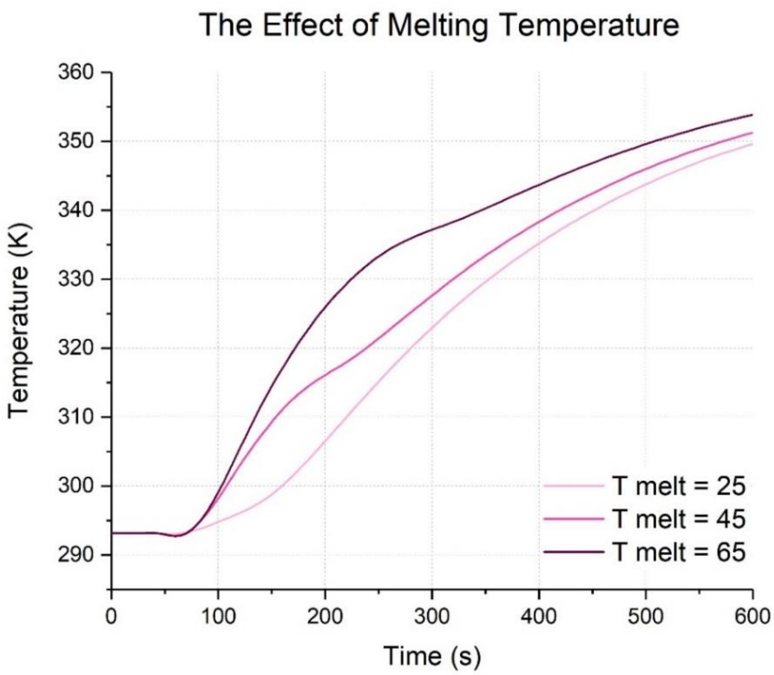

Fig. 2: Effect of the melting temperature on the heating dynamics.

Figures 3 and 4 present work with parameters which change before and after the phase change. These are the thermal conductivity and the specific heat capacity, respectively. From Figure 3, results indicate that the higher the thermal conductivity of the liquid, the higher the final temperature reached by the spheres. This is denoted in the almost horizontal lines in the contour diagram and the heavy blue section at the bottom of the chart, which show that the effect of the thermal conductivity of the solid plays a very limited part in the final temperature outcome. The highest temperatures reached are approximately 360K, whereas the minimum values were around 330K. This 30K difference really proves how the thermal conductivity of the liquid greatly influences the outcome of the final temperature and can delay the charging time if the values remain too low. However, looking at the thermal conductivity of the solid, the maximum difference would not be more than 5K. High liquid values were close to reaching the temperature of the HTF, where the temperature increase of the centre sphere is a value of 66.85K (360K – 293.15K), yet high solid values struggled with a smaller increase of 36.85K (330K – 293.15K).

Figure 4 shows a similar, yet opposite, trend. It suggests that the higher the value of the specific heat capacity of the liquid, the lower the final temperature the spheres will reach. This suggests that the system will charge fastest when the liquid value is at its lowest. Again, the idea that the liquid parameters have a heavier influence over the system is denoted in these near to horizontal lines and the heavy read area at the bottom of the graph, indicating that the solid counterpart is not affecting the system to that extent. Nonetheless, it is worth noting that the specific heat of the solid does show lines slanting down much more visibly than the thermal conductivity ones. This portrays the idea that the specific heat capacity of the solid is more influential over the final temperature than the thermal conductivity of the solid was for its counterpart, and that high specific heat capacity of the solid values ultimately will results in a higher temperature. Maximum temperatures reached by these tests are similar to the ones in Figure 3 at approximately 361K, but the minimum values are significantly higher at roughly 350K. This difference of only 11K, as opposed to the previous 30K, suggests that the effect of the specific heat capacity is not as influential for the charging time of the system as the thermal conductivity is.

The contour diagram plotted in Figure 5 shows the effect of the latent heat and density in terms of heat absorption per sphere. This diagram clearly demonstrates that both high latent heat and density will positively maximise the heat absorption per sphere.

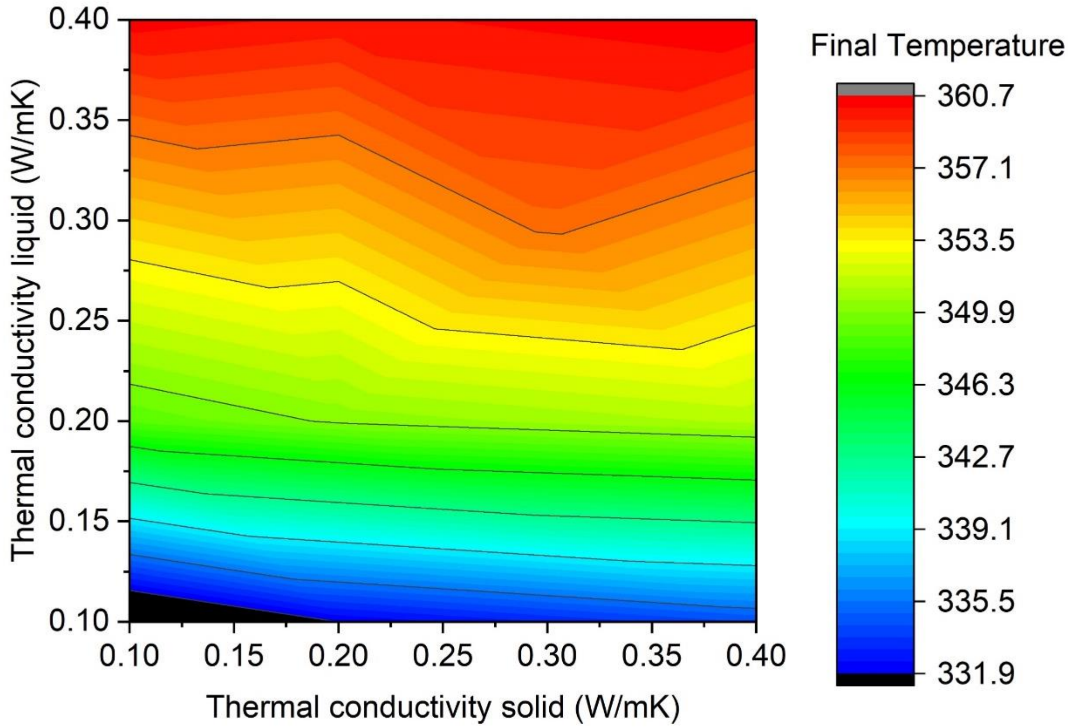

Fig. 3: Contour plot of thermal conductivity of the solid vs thermal conductivity of the liquid.

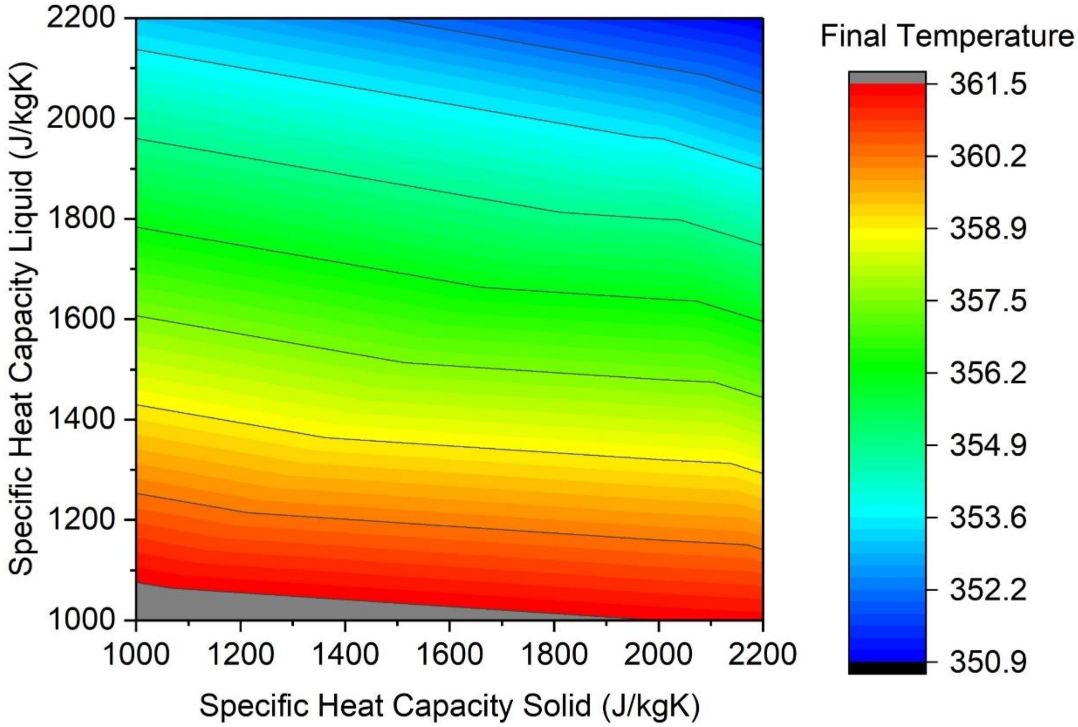

Fig. 4: Contour plot of specific heat capacity of the solid vs specific heat capacity of the liquid.

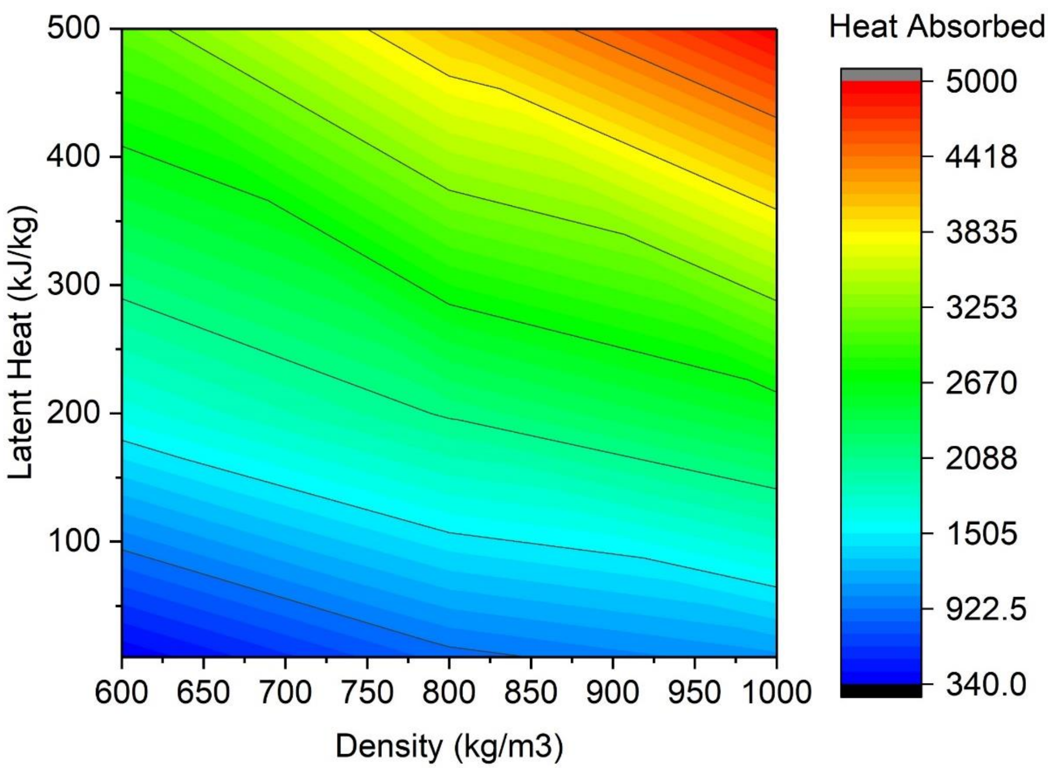

Fig. 5: Contour plot of specific heat capacity of latent heat vs density.

4. Conclusion

A 2D numerical simulation on a packed bed storage for user-defined materials was done in the software COMSOL Multiphysics. The study focused on finding relevant parameters and how they affect this type of system design. Finally, results summarise that:

- Low specific heat capacity of the liquid and high thermal conductivity of the liquid positively influence max charging temperatures; a similar effect is observed for low density values.
- High density and latent heat are beneficial for maximum heat absorption.
- Specific heat capacity and thermal conductivity of the liquid are more influential than those of the solid.

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